Heat and solute transport

Prof. Gabriele Manoli
gabriele.manoli@epfl.ch

Today's Lecture (if time allows…)

- **Introduction to:**
    - **heat transport** in porous media
    - **solute transport** in porous media
- "It's time for coffee"!

Continuity equation

The conservation (or continuity) equation states that the temporal variation of the variable considered (water content, density of heat, concentration, etc.) is equal to the spatial variation of the flow, corrected for possible contributions, losses or transformations within the system

General Form:

$$\boxed{\frac{\partial \rho}{\partial t} = -\nabla \cdot \boldsymbol{q} + \sum\nolimits_i r_i}$$

ρ = Volumetric concentration of the variable considered

q = flux across the system boundaries

r_i = rate of production, degradation, or transfromation within the domain (many sources/sinks *i* may exist)

Sustance	ρ	Unit	$\boldsymbol{q}$	Unit
Water	Water content, θ	$m^3\ m^{-3}$	Darcy’s law	$m\ s^{-1}$
Heat	Quantity of heat	$J\ m^{-3}$	Fourier’s law	$J\ m^{-2}\ s^{-1}$
Chemical substance or gas	Concentration	$kg\ m^{-3}$	Fick’s law	$kg\ m^{-2}\ s^{-1}$

Heat transport

The **first law of heat conduction**, known as **Fourier's law**, states that the flux of heat in a homogeneous body is in the direction of, and proportional to, the temperature gradient:

$$\boldsymbol{q}_h = -K_h \nabla T$$

to account for nonsteady (transient) conditions, we invoke the principle of **energy conservation** in the form of the **continuity equation**, stating that, in the absence of internal sources or sinks of heat, the time rate of change in heat content of a volume element must equal the change of flux with distance:

$$\rho c_m \frac{\partial T}{\partial t} = -\nabla \cdot \boldsymbol{q}_h$$

where ρ is mass density and c_m specific heat capacity per unit mass (defined as the change in heat content of a unit mass of the body per unit change in temperature). The product $C=\rho c_m$ is the **specific heat capacity** per unit volume

Note: $\mathrm{E} = \rho c_m T$ is the thermal energy

Heat transport

Combining the previous two equations we obtain the desired **second law of heat conduction**:

$$\boxed{C\frac{\partial T}{\partial t} = \nabla \cdot (K_h \nabla T)}$$

Introducing the therma diffusivity $D_h = K_h/\rho c_m$ and assuming it is a constant, leads to:

$$\frac{\partial T}{\partial t} = D_h \nabla^2 T$$

To solve the foregoing equations so as to obtain a description of how temperature varies in space and time, we need to know, by measurement or calculation, the pertinent values of the three parameters just defined, namely, the volumetric heat capacity *C*, thermal conductivity *K*, and/or thermal diffusivity *D*. Together, they are called the **thermal properties of soils**.

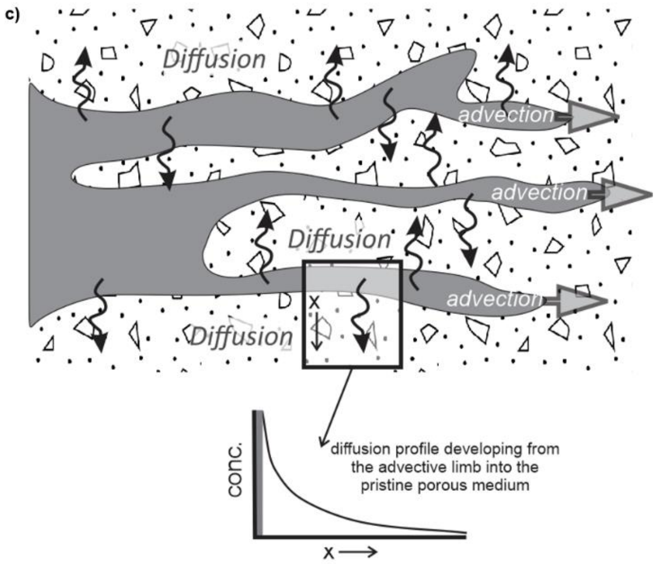
Solute transport

The **conservation of mass** for a **solute dissolved in water** is (assuming non-reactive transport):

$$\frac{\partial(C_s\theta)}{\partial t} = -\nabla \cdot \boldsymbol{q}_s$$

Solute movement can occur via three mechanisms: mass flow (**advection**), molecular **diffusion**, and hydrodynamic **dispersion**, i.e.

$$\boldsymbol{q}_s = \boldsymbol{q}_{s,adv} + \boldsymbol{q}_{s,diff} + \boldsymbol{q}_{s,disp}$$



https://books.gw-project.org/groundwater-velocity/chapter/subsurface-mixing/

Solute transport

- **Advection** (or mass flow) of soil water, sometimes called the Darcian flow, carries with it a flux of solutes $\boldsymbol{q}_{s,adv}$ proportional to their concentration C_s:

$$\boldsymbol{q}_{s,adv} = \boldsymbol{q}C_s = \overline{\boldsymbol{v}}\theta C_s \qquad \text{where} \qquad \boldsymbol{q} = -K\nabla(h+z)$$

- **Diffusion** processes commonly occur within multicomponent gaseous or liquid phases, in consequence of the random thermal motion (often called Brownian motion) and repeated collisions and deflections of molecules in the fluid. Solutes tend to diffuse from zones where their concentration is higher to where it is lower. In bulk water at rest, the rate of diffusion $\boldsymbol{q}_{s,diff}$ is related by **Fick's first law** to the gradient of the concentration C_s :

$$\boldsymbol{q}_{s,diff} = -D_{diff}\nabla C_s$$

where D_{diff} is the diffusion coefficient

- **Hydrodynamic dispersion** results from the microscopic nonuniformity of flow velocity in the soil's conducting pores. This differs from diffusion in its mechanism but tends to produce an analogous tendency to mix and eventually to even-out the differences in concentration:

$$\boldsymbol{q}_{s,disp} = -D_{disp}\nabla C_s$$

where D_{disp} is the dispersion coefficient

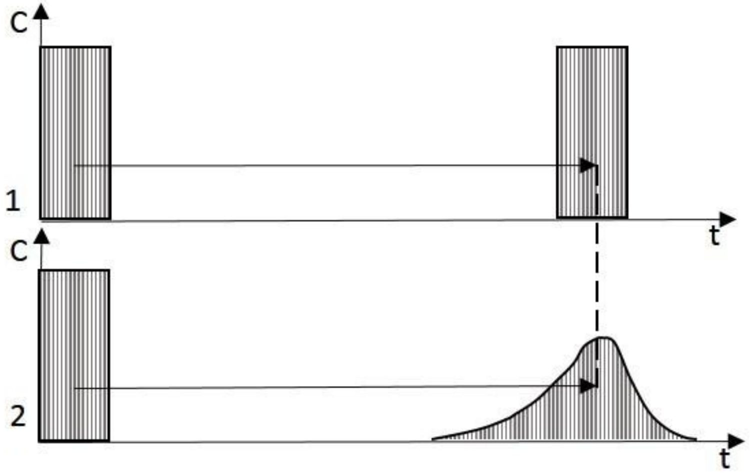
Solute transport

The **conservation of mass** for a solute dissolved in water thus become

$$\frac{\partial(C_s\theta)}{\partial t} = -\nabla\cdot\boldsymbol{q}_s \qquad \text{with} \qquad \boldsymbol{q}_s = \overline{\boldsymbol{v}}\theta C_s - D_{diff}\nabla C_s - D_{disp}\nabla C_s$$

Since in practice the diffusion and dispersion phenomena cannot be separated, we can write the advection-dispersion equation in the following form:

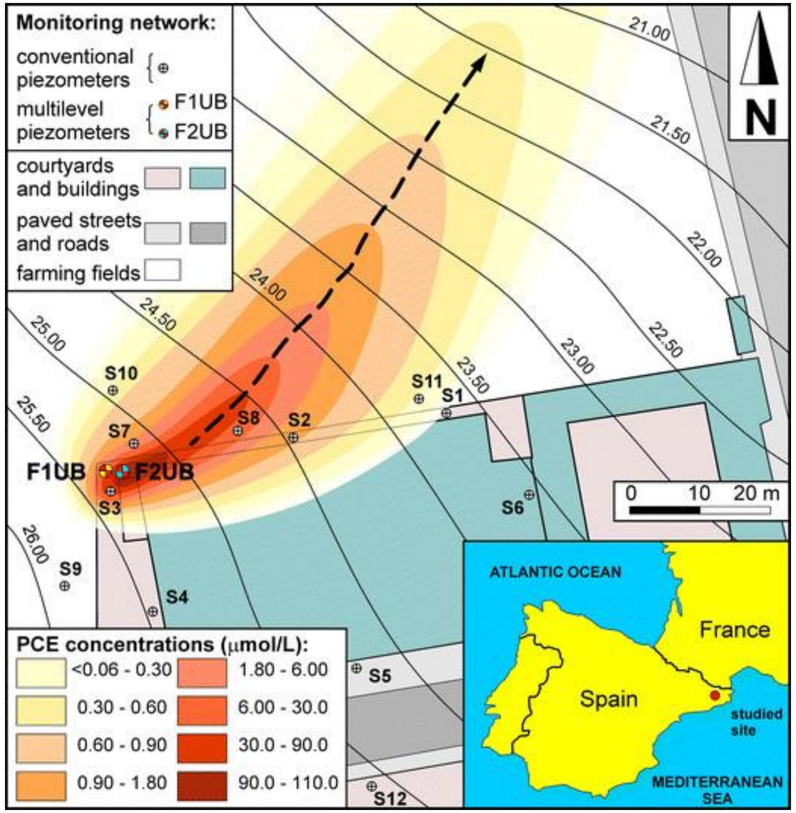
$$\boxed{\frac{\partial C_s}{\partial t} = -\nabla\cdot(\overline{\boldsymbol{v}}C_s) + \nabla\cdot(D_d\nabla C_s)}$$



Saatsaz and Eslamian (2020)

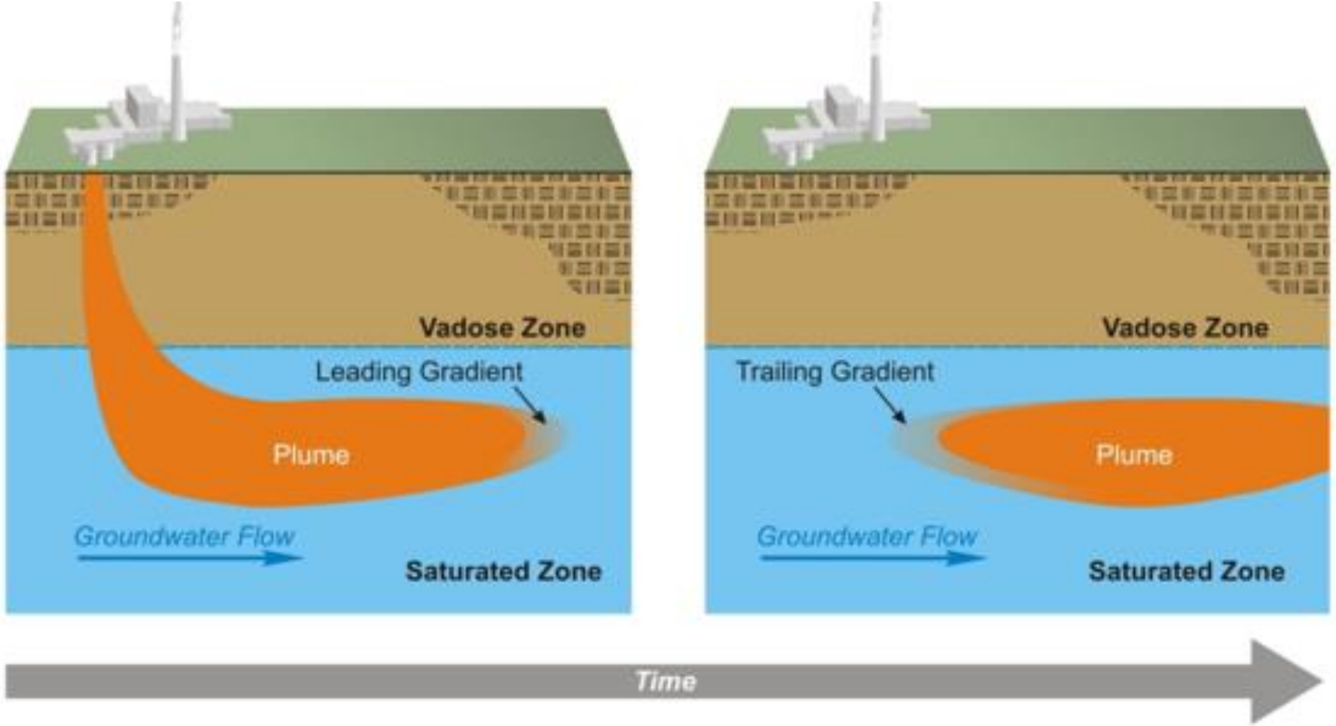
Where D_d is the lumped diffusion–dispersion coefficient

Solute transport



Puigserver et al. (2020)

Solute transport



https://www.enviro.wiki/

Is it time for coffee?

https://neurosciencenews.com/espresso-alzheimers-23657/

Almost!

Just a final recap of (soil physics) theory first!

It’s time for coffee!

https://neurosciencenews.com/espresso-alzheimers-23657/

Article

Systematically Improving Espresso: Insights from Mathematical Modeling and Experiment

Michael I. Cameron,[1,10] Dechen Morisco,[1,10] Daniel Hofstetter,[2] Erol Uman,[3] Justin Wilkinson,[4] Zachary C. Kennedy,[5] Sean A. Fontenot,[8] William T. Lee,[6,7] Christopher H. Hendon,[8,11,*] and Jamie M. Foster[9,*]

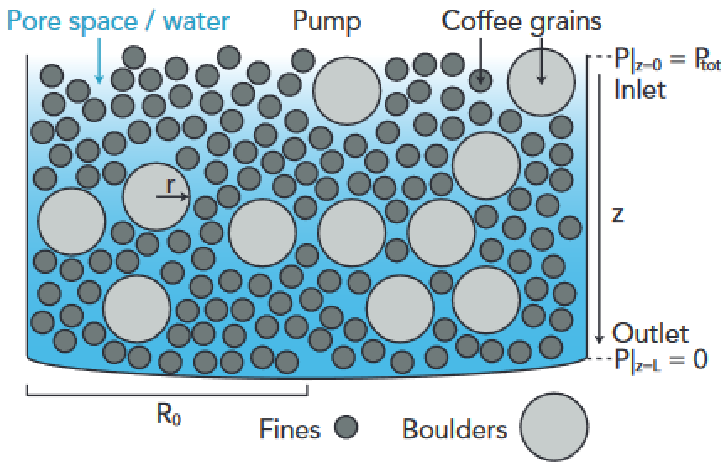


Figure 1. A Schematic of the Espresso Basket Geometry

The coffee grounds are shown in gray (Ω_s), and the pore space, which is filled with water during extraction, is shown in blue (Ω_l). The macroscopic spatial coordinate measuring depth through the bed, z, the microscopic spatial coordinate measuring radial position within the spherical coffee particles, r, as well as the basket radius, R_0, are also indicated.

Cameron et al (2019)

It’s time for coffee!

Modeling Mass and Heat Transfer in Multiphase Coffee Aroma Extraction

David Beverly, Estefanía Lopez-Quiroga, Robert Farr, John Melrose, Sian Henson, Serafim Bakalis, and Peter J. Fryer*

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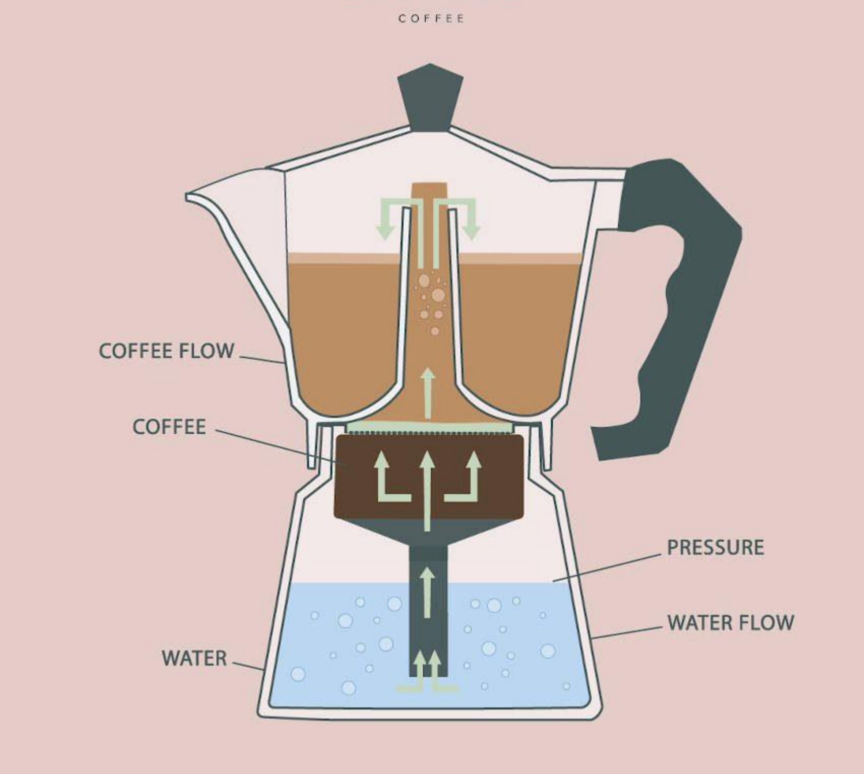
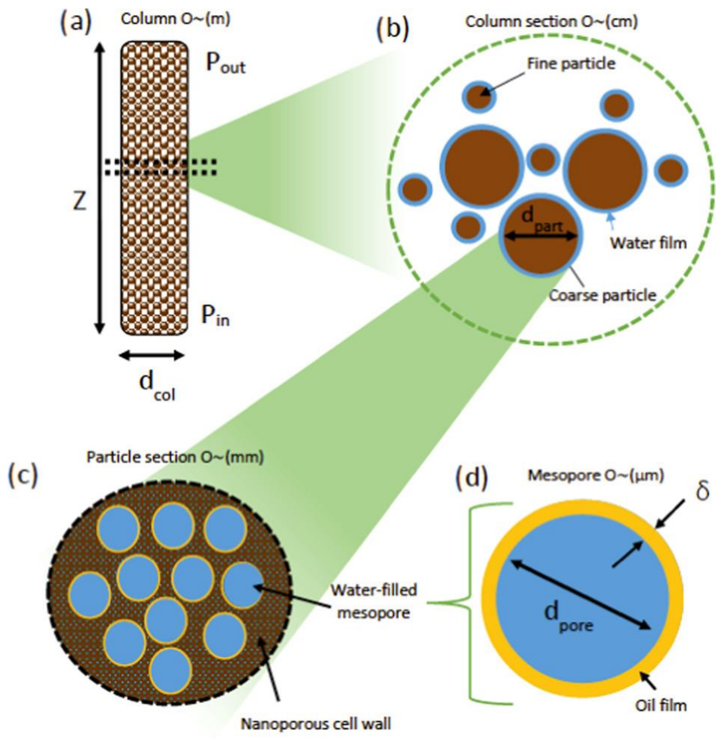


https://balancecoffee.co.uk/blogs/



Beverly et al (2020)

It’s time for coffee!

Modelling of coffee extraction during brewing using multiscale methods: An experimentally validated model

K.M. Moroney [a,*], W.T. Lee [a], S.B.G. O'Brien [a], F. Suijver [b], J. Marra [b]

[a] MACSI, Department of Mathematics and Statistics, University of Limerick, Ireland
[b] Philips Research, Eindhoven, The Netherlands

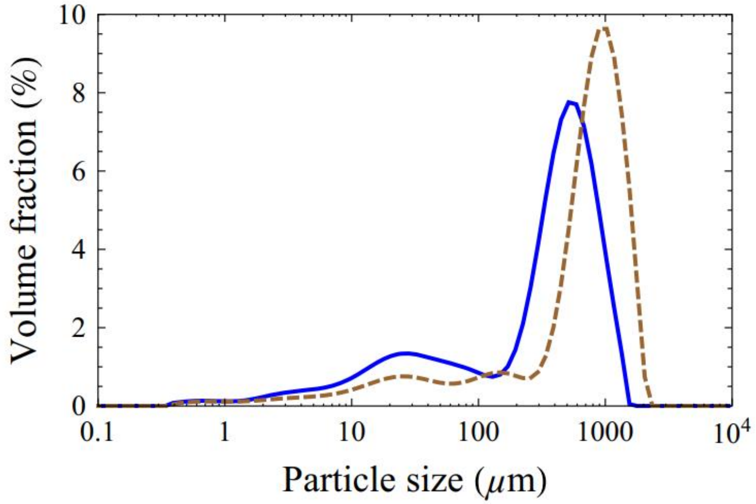


Fig. 1. Coffee grind size distributions for JK standard drip filter grind (–) and Cimbali #20 grind (- -). Distributions are expressed in terms of volume fraction percentages of particles of a given diameter.

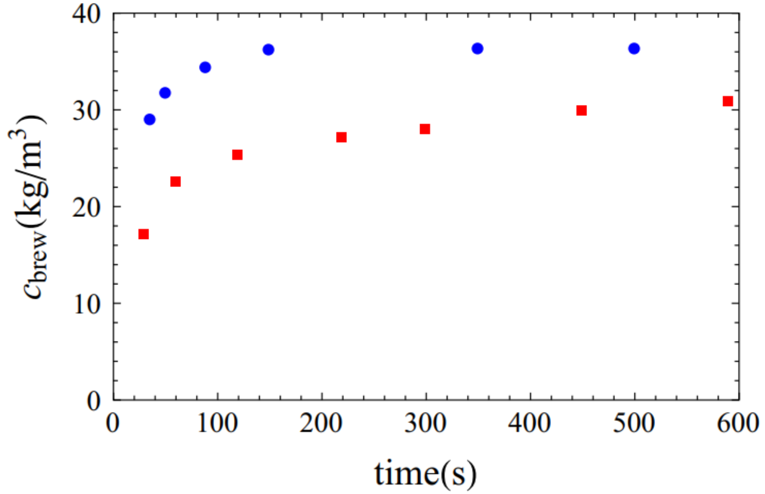
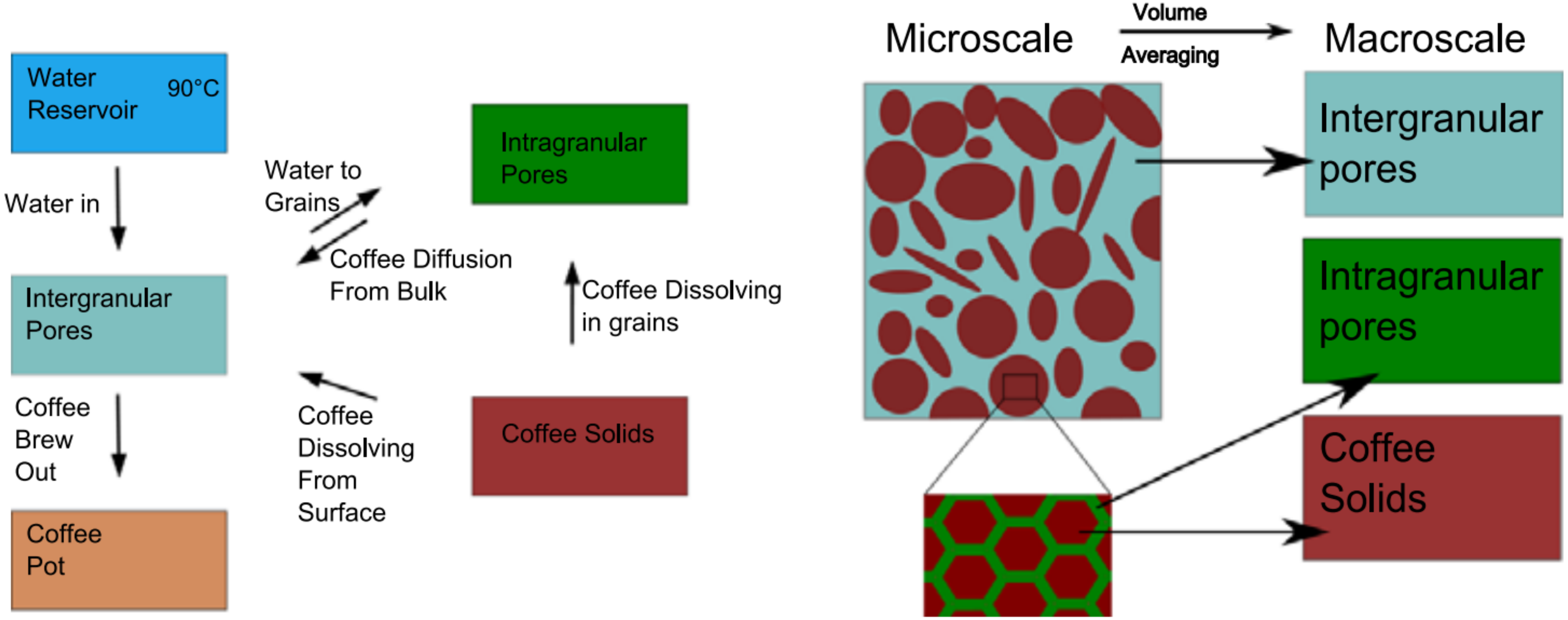


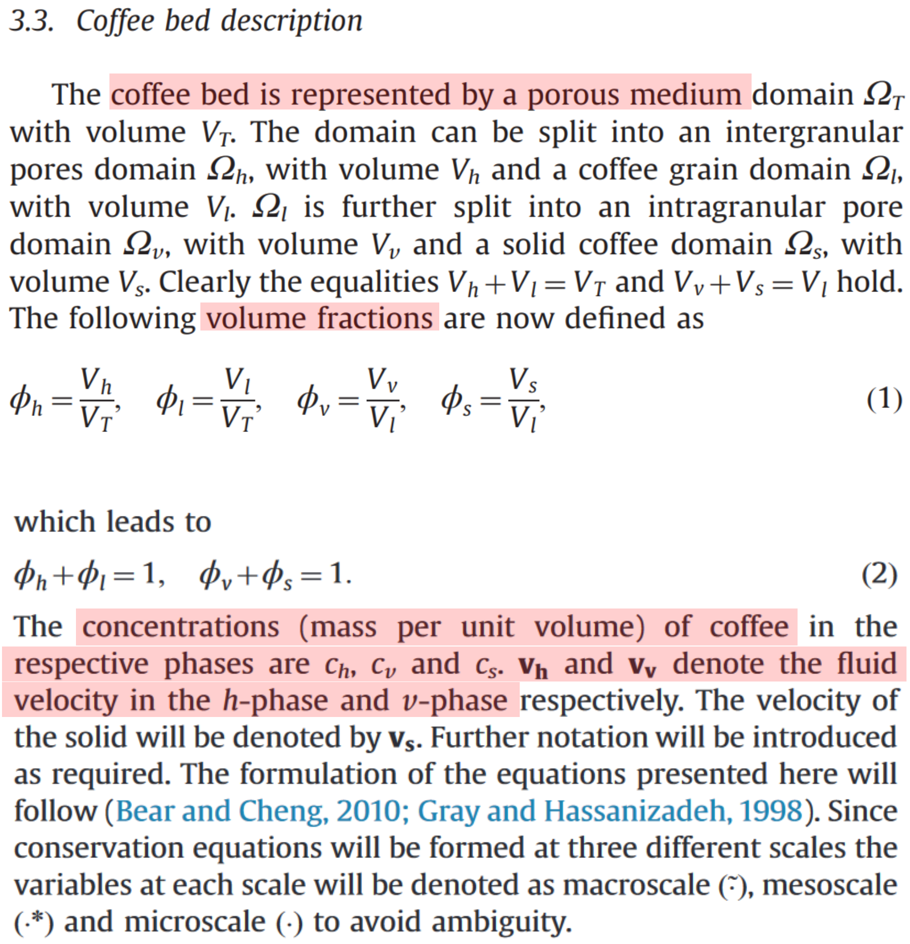
Fig. 2. Coffee solubles concentration profiles for JK standard drip filter grind (●) and Cimbali #20 grind (□) during batch extraction experiments. In these experiments 60 g of coffee with approximately 4% moisture was mixed with 0.5 l of hot water in a French press type cylinder.

It’s time for coffee!



Moroney et al (2015)

It’s time for coffee!



3.3. *Coffee bed description*

The coffee bed is represented by a porous medium domain Ω_T with volume V_T. The domain can be split into an intergranular pores domain Ω_h, with volume V_h and a coffee grain domain Ω_l, with volume V_l. Ω_l is further split into an intragranular pore domain Ω_v, with volume V_v and a solid coffee domain Ω_s, with volume V_s. Clearly the equalities $V_h + V_l = V_T$ and $V_v + V_s = V_l$ hold. The following volume fractions are now defined as

$$\phi_h = \frac{V_h}{V_T}, \quad \phi_l = \frac{V_l}{V_T}, \quad \phi_v = \frac{V_v}{V_l}, \quad \phi_s = \frac{V_s}{V_l}, \tag{1}$$

which leads to

$$\phi_h + \phi_l = 1, \quad \phi_v + \phi_s = 1. \tag{2}$$

The concentrations (mass per unit volume) of coffee in the respective phases are c_h, c_v and c_s. $\mathbf{v_h}$ and $\mathbf{v_v}$ denote the fluid velocity in the h-phase and v-phase respectively. The velocity of the solid will be denoted by $\mathbf{v_s}$. Further notation will be introduced as required. The formulation of the equations presented here will follow (Bear and Cheng, 2010; Gray and Hassanizadeh, 1998). Since conservation equations will be formed at three different scales the variables at each scale will be denoted as macroscale $(\tilde{\cdot})$, mesoscale $(\cdot^*)$ and microscale $(\cdot)$ to avoid ambiguity.

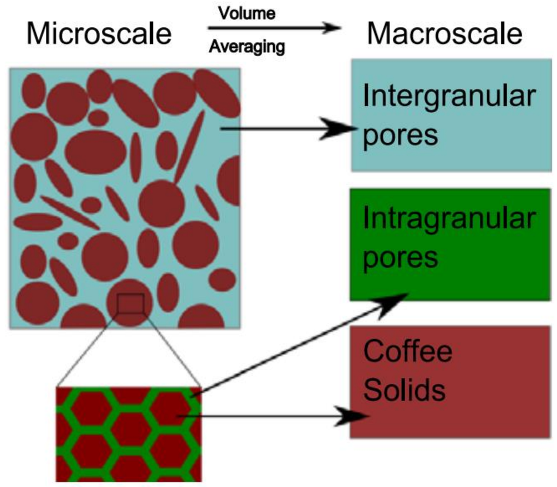


Fig. 4. Macroscale equations are matched to microscale equations using volume averaging. At a macroscopic level the system is represented by three overlapping continua for the intergranular pores (h-phase), intragranular pores (v-phase) and solid coffee (s-phase).

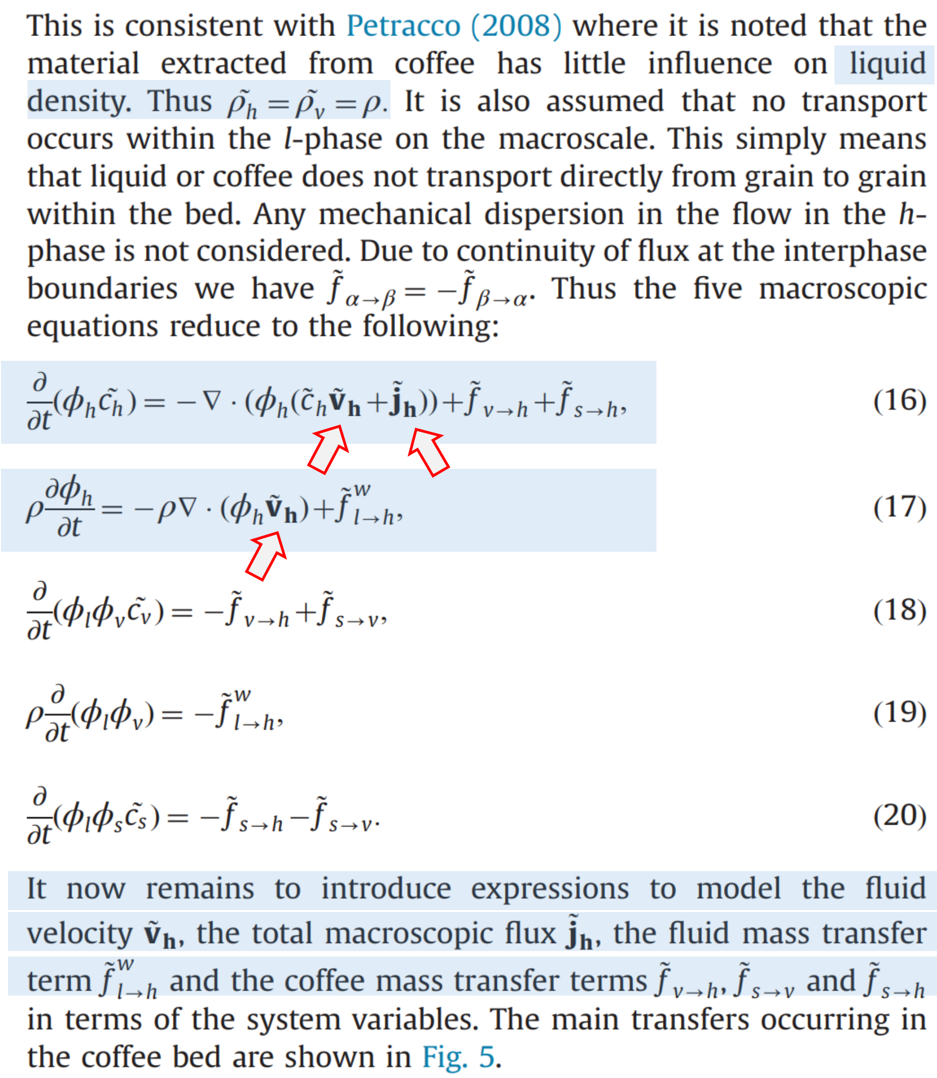
h-phase

s-phase

v-phase

Moroney et al (2015)

It’s time for coffee!



This is consistent with Petracco (2008) where it is noted that the material extracted from coffee has little influence on liquid density. Thus $\tilde{\rho}_h = \tilde{\rho}_v = \rho$. It is also assumed that no transport occurs within the l-phase on the macroscale. This simply means that liquid or coffee does not transport directly from grain to grain within the bed. Any mechanical dispersion in the flow in the h-phase is not considered. Due to continuity of flux at the interphase boundaries we have $\tilde{f}_{\alpha\to\beta} = -\tilde{f}_{\beta\to\alpha}$. Thus the five macroscopic equations reduce to the following:

Coffee:

$$\frac{\partial}{\partial t}(\phi_h\tilde{c}_h) = -\nabla\cdot(\phi_h(\tilde{c}_h\tilde{\mathbf{v}}_{\mathbf{h}}+\tilde{\mathbf{j}}_{\mathbf{h}}))+\tilde{f}_{v\to h}+\tilde{f}_{s\to h}, \tag{16}$$

Water:

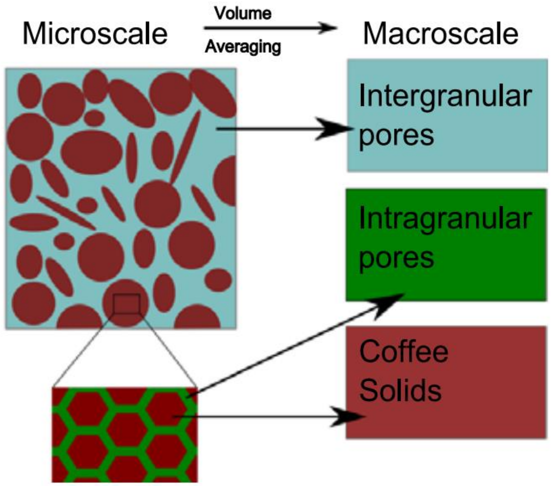
$$\rho\frac{\partial\phi_h}{\partial t} = -\rho\nabla\cdot(\phi_h\tilde{\mathbf{v}}_{\mathbf{h}})+\tilde{f}^{w}_{l\to h}, \tag{17}$$

$$\frac{\partial}{\partial t}(\phi_l\phi_v\tilde{c}_v) = -\tilde{f}_{v\to h}+\tilde{f}_{s\to v}, \tag{18}$$

$$\rho\frac{\partial}{\partial t}(\phi_l\phi_v) = -\tilde{f}^{w}_{l\to h}, \tag{19}$$

$$\frac{\partial}{\partial t}(\phi_l\phi_s\tilde{c}_s) = -\tilde{f}_{s\to h}-\tilde{f}_{s\to v}. \tag{20}$$

It now remains to introduce expressions to model the fluid velocity $\tilde{\mathbf{v}}_{\mathbf{h}}$, the total macroscopic flux $\tilde{\mathbf{j}}_{\mathbf{h}}$, the fluid mass transfer term $\tilde{f}^{w}_{l\to h}$ and the coffee mass transfer terms $\tilde{f}_{v\to h}$, $\tilde{f}_{s\to v}$ and $\tilde{f}_{s\to h}$ in terms of the system variables. The main transfers occurring in the coffee bed are shown in Fig. 5.



h-phase

s-phase

v-phase

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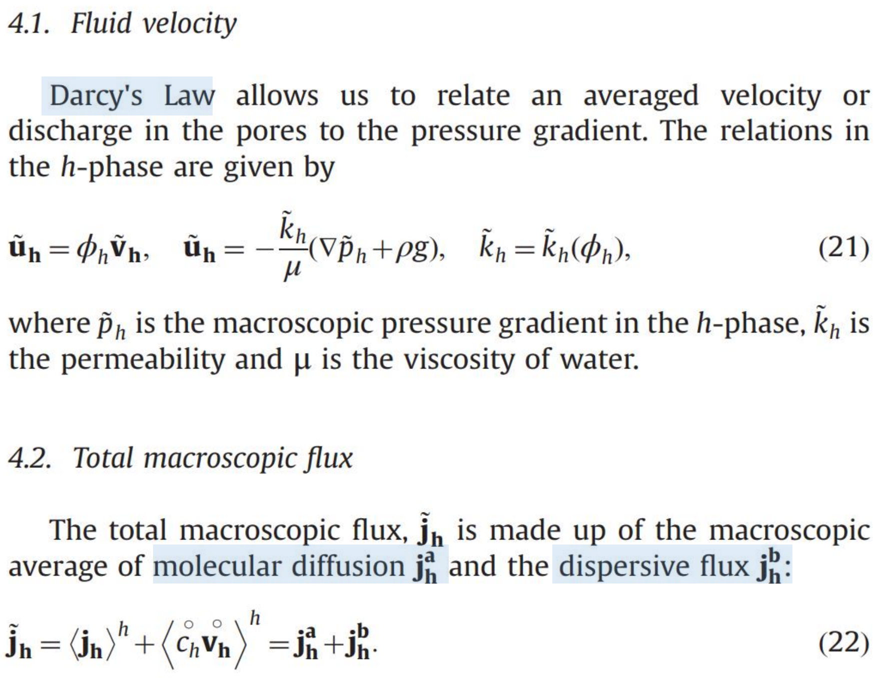
Moroney et al (2015)

It’s time for coffee!



4.1. Fluid velocity

Darcy's Law allows us to relate an averaged velocity or discharge in the pores to the pressure gradient. The relations in the *h*-phase are given by

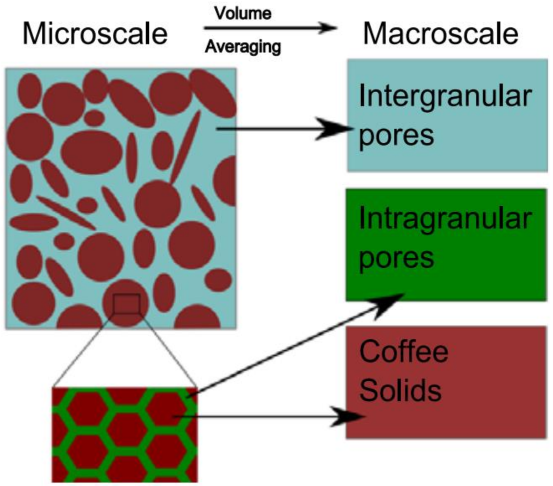
$$\tilde{\mathbf{u}}_{\mathbf{h}} = \phi_h \tilde{\mathbf{v}}_{\mathbf{h}}, \quad \tilde{\mathbf{u}}_{\mathbf{h}} = -\frac{\tilde{k}_h}{\mu}(\nabla \tilde{p}_h + \rho g), \quad \tilde{k}_h = \tilde{k}_h(\phi_h), \tag{21}$$

where $\tilde{p}_h$ is the macroscopic pressure gradient in the *h*-phase, $\tilde{k}_h$ is the permeability and μ is the viscosity of water.

4.2. Total macroscopic flux

The total macroscopic flux, $\tilde{\mathbf{j}}_{\mathbf{h}}$ is made up of the macroscopic average of molecular diffusion $\mathbf{j}_{\mathbf{h}}^{\mathbf{a}}$ and the dispersive flux $\mathbf{j}_{\mathbf{h}}^{\mathbf{b}}$:

$$\tilde{\mathbf{j}}_{\mathbf{h}} = \langle \mathbf{j}_{\mathbf{h}} \rangle^h + \left\langle \mathring{c}_h \mathring{\mathbf{v}}_{\mathbf{h}} \right\rangle^h = \mathbf{j}_{\mathbf{h}}^{\mathbf{a}} + \mathbf{j}_{\mathbf{h}}^{\mathbf{b}}. \tag{22}$$



h-phase

s-phase

v-phase

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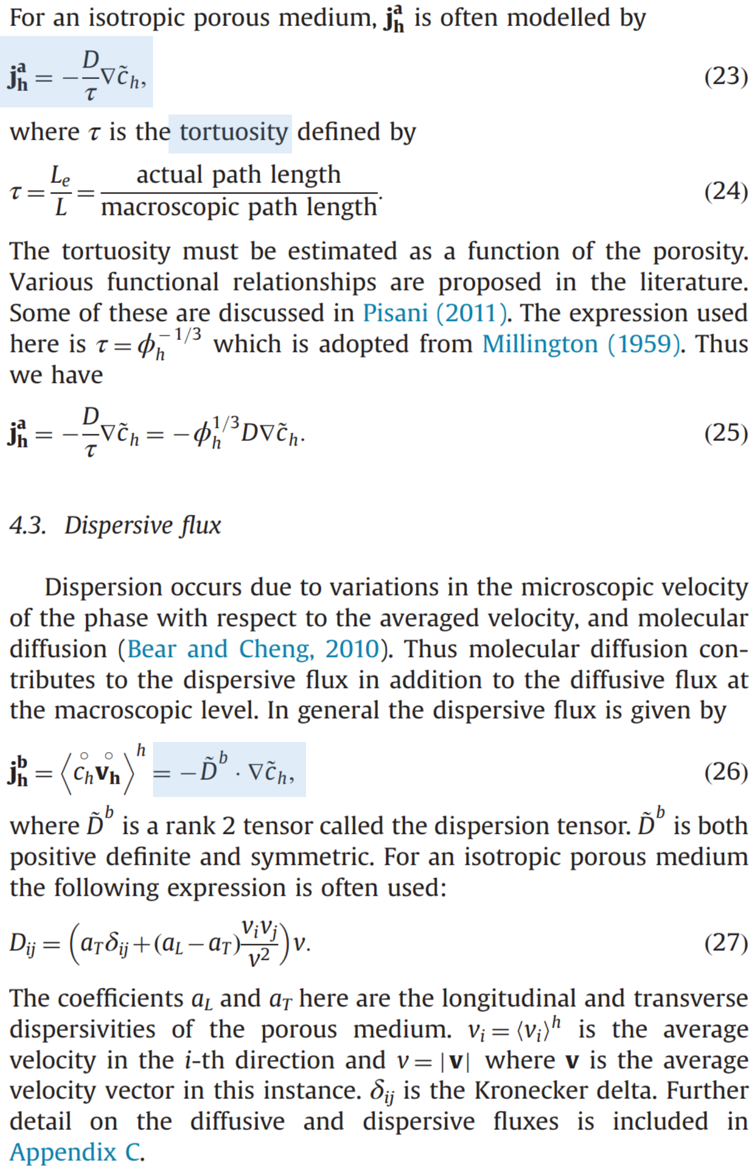
Moroney et al (2015)

It’s time for coffee!



For an isotropic porous medium, $\mathbf{j}_h^a$ is often modelled by

$$\mathbf{j}_h^a = -\frac{D}{\tau}\nabla\tilde{c}_h, \tag{23}$$

where τ is the tortuosity defined by

$$\tau = \frac{L_e}{L} = \frac{\text{actual path length}}{\text{macroscopic path length}}. \tag{24}$$

The tortuosity must be estimated as a function of the porosity. Various functional relationships are proposed in the literature. Some of these are discussed in Pisani (2011). The expression used here is $\tau = \phi_h^{-1/3}$ which is adopted from Millington (1959). Thus we have

$$\mathbf{j}_h^a = -\frac{D}{\tau}\nabla\tilde{c}_h = -\phi_h^{1/3} D\nabla\tilde{c}_h. \tag{25}$$

4.3. Dispersive flux

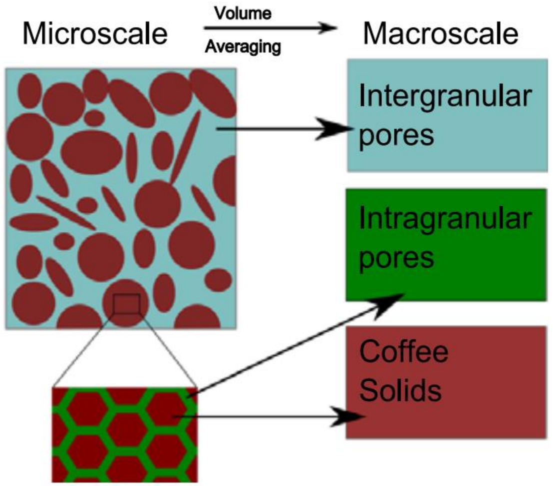
Dispersion occurs due to variations in the microscopic velocity of the phase with respect to the averaged velocity, and molecular diffusion (Bear and Cheng, 2010). Thus molecular diffusion contributes to the dispersive flux in addition to the diffusive flux at the macroscopic level. In general the dispersive flux is given by

$$\mathbf{j}_h^b = \left\langle \mathring{c}_h \mathring{\mathbf{v}}_h \right\rangle^h = -\tilde{D}^b \cdot \nabla\tilde{c}_h, \tag{26}$$

where $\tilde{D}^b$ is a rank 2 tensor called the dispersion tensor. $\tilde{D}^b$ is both positive definite and symmetric. For an isotropic porous medium the following expression is often used:

$$D_{ij} = \left(a_T\delta_{ij} + (a_L - a_T)\frac{v_i v_j}{v^2}\right)v. \tag{27}$$

The coefficients a_L and a_T here are the longitudinal and transverse dispersivities of the porous medium. $v_i = \langle v_i \rangle^h$ is the average velocity in the i-th direction and $v = |\mathbf{v}|$ where $\mathbf{v}$ is the average velocity vector in this instance. δ_{ij} is the Kronecker delta. Further detail on the diffusive and dispersive fluxes is included in Appendix C.



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Moroney et al (2015)

It’s time for coffee!

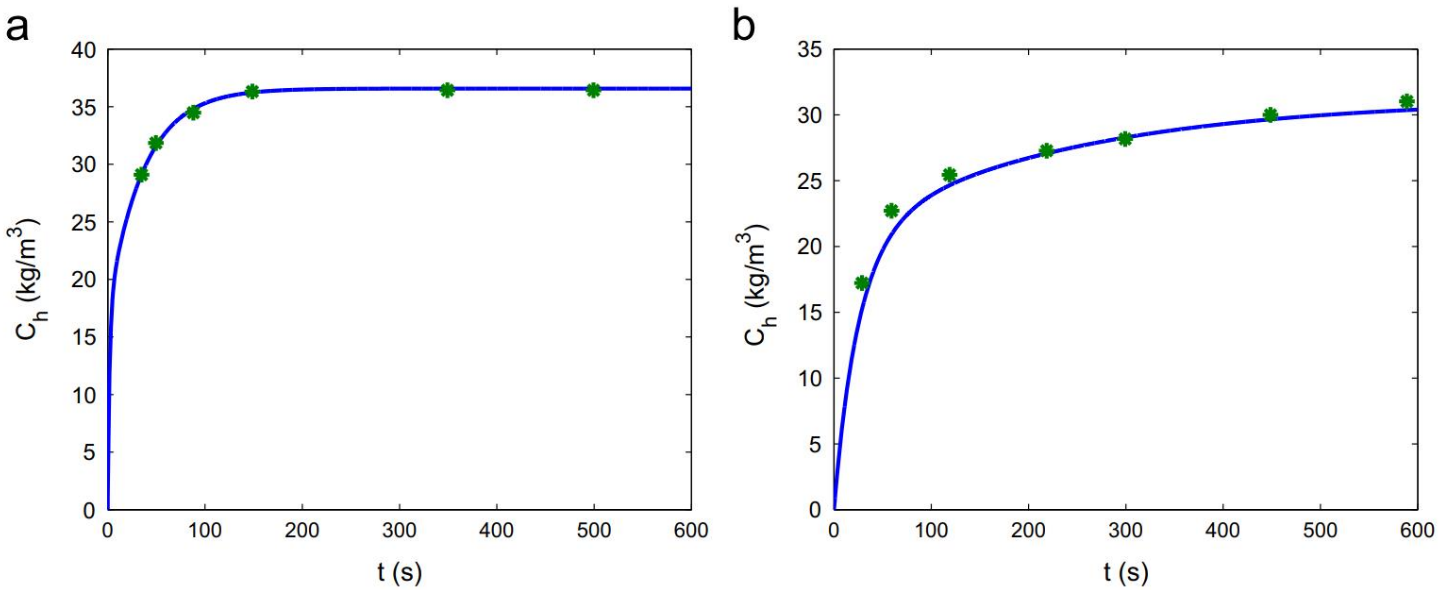


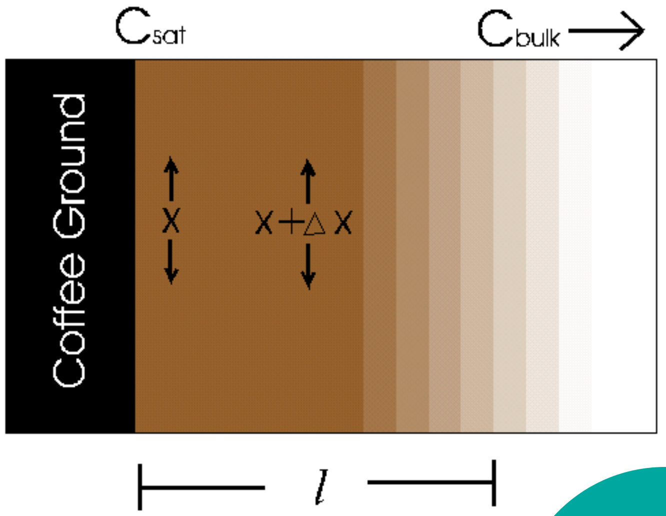
Fig. 6. Comparison between numerical solution (–) with parameters from Table 1 and experiment (∗) for the batch extraction experiments for (a) JK drip filter grind and (b) Cimbali #20 grind.

Moroney et al (2015)

It's time for coffee!

We are now going to use Fick's law to perform a measurement to find the rate of accumulation of caffeine in brewing coffee. Along the way, we will discover why it is important to grind coffee beans before you brew them.

- *D* = 1.14 * 10-4 m2/sec (caffeine and water)
- C_{sat} = 1.77 mol caffeine / mol water is the maximum concentration of caffeine that may be contained in water. For water at the brewing temperature of coffee,
- C_{bulk} = 0.538 mol caffeine / mol water is the average concentration of caffeine in the final product, a cup of coffee..
- *l* is the distance between the surface of the coffee ground and the bulk coffee at concentration C_{bulk}. This is a stagnant layer of liquid next to the surface of the coffee ground. We can estimate the distance to be 0.00001 m.



https://uweb.engr.arizona.edu/~blowers/cooking/mass/coffee2.html

Self-Study

It's time for coffee!

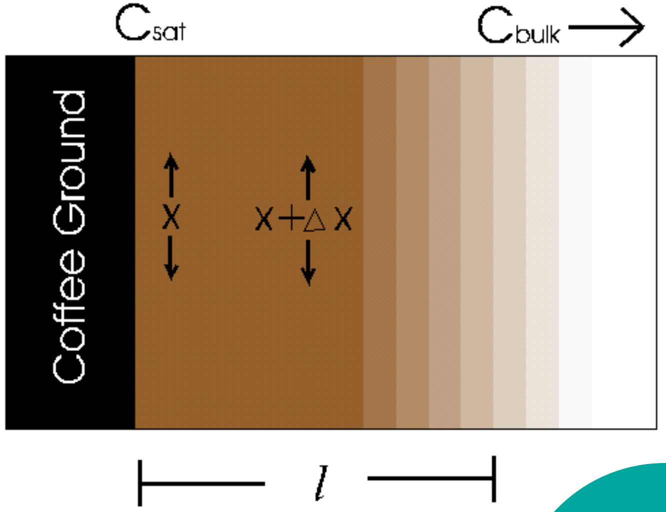
$$J = D\frac{C_{sat} - C_{bulk}}{l} \Rightarrow J = 1.14 \times 10^{-4}\frac{1.77 - 0.538}{0.00001} = 14 \left[\frac{mol\, caffeine}{s\, m^2}\right]$$

The amount of caffeine produced per time is therefore directly related to the surface area of the coffee ground. If we double the size of the surface area of the coffee ground, we halve the time it takes to brew. Grinding the the coffee increases the surface area of the coffee tremendously.

Can you imagine the time it would take to brew coffee from whole beans?

- If we take a coffee bean to have roughly 1 $cm^2 = 10^{-4}$ m^2 surface area and assume that about 200 coffee beans are used to brew a pot of coffee, we find that they have an initial surface area of 0.02 m^2.
- After grinding, the same coffee beans become a coarse powder with a surface area of about 800 m^2 - an increase of 40'000%!

If it takes only one second of contact between the water and the contact between the water and the ground coffee, it would take 40'000 more seconds to brew a pot of coffee from beans than from coffee powder - that's over 11 hours!



https://uweb.engr.arizona.edu/~blowers/cooking/mass/coffee2.html

Self-Study

This week exercises & assignments

- **Exercises:** additional problems (optional) + time to finish previous exercises/questions on course material
- **Computer Lab:** free time to finalize report
- Report submission:
    - submit your computer lab report (1 per group) in Moodle.
    - Deadline: **December 6th at 23h59**

Useful links

- **Solute transport:**
  - Transport Equations in porous media
  - Mechanisms of solute transport in soils (Youtube)

- **Modeling coffee:**
  - Modelling of coffee extraction during brewing using multiscale methods
  - Systematically Improving Espresso
  - Modeling Mass and Heat Transfer in Multiphase Coffee Aroma Extraction