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Comparison of Heat and Mass Transport at the Micro-Scale

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Phenomena of heat and mass transfer are often compared, in various porous media applications. Questions of practical interest are, for example, if tracers can be used for the prediction of heat flow, or vice versa if heat can be utilized as, possibly retarded, tracer for predicting the migration of contaminants, nutrients or other substances. Using numerical modelling in artificial porous media we compute heat and mass transport for pore length scales in the range of micrometers. The simulations show different behaviour for heat and for mass, which is due to the different values of the relevant parameters (high Lewis number) and the different physics of transport in the solid phase.

Differences between Heat & Mass Transfer

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Mass Transport

in fluid phase

- Diffusion
- Dispersion
- Sorption
- Decay / Degradation
- Production / Consumption
- Dissolution / Precipitation
- Kinetics

in solid phase

- Matrix diffusion (?)

Heat Transport

in fluid phase

- Diffusion
- Dispersion (?)
- Production / Consumption

in solid phase

- Diffusion

Modelling Approach

COMSOL MULTIPHYSICS

- Solution of ***Navier-Stokes*** equations in pore space (stationary)
  - No slip boundary condition at pore surfaces
  - Pressure gradient prescribed

- ***Advection-diffusion*** mode for mass transport in pore space (transient)
  - Molecular diffusivity
  - Concentration specified at inflow

- ***Convection-conduction*** mode for heat transport in pore space and in porous medium (two sub-domains, transient)
  - Temperature specified at inflow

Density & Viscosity Effects

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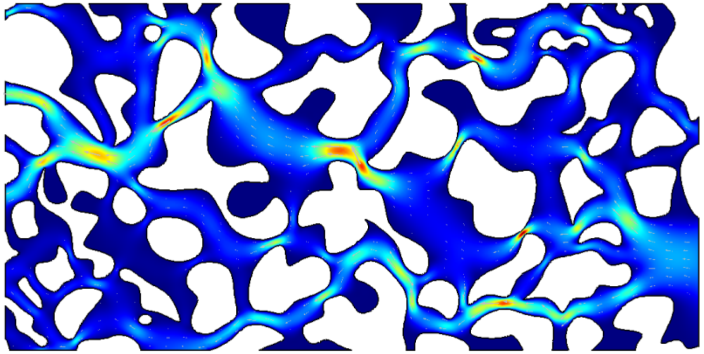
Additional effects according to this coupling could emerge due to

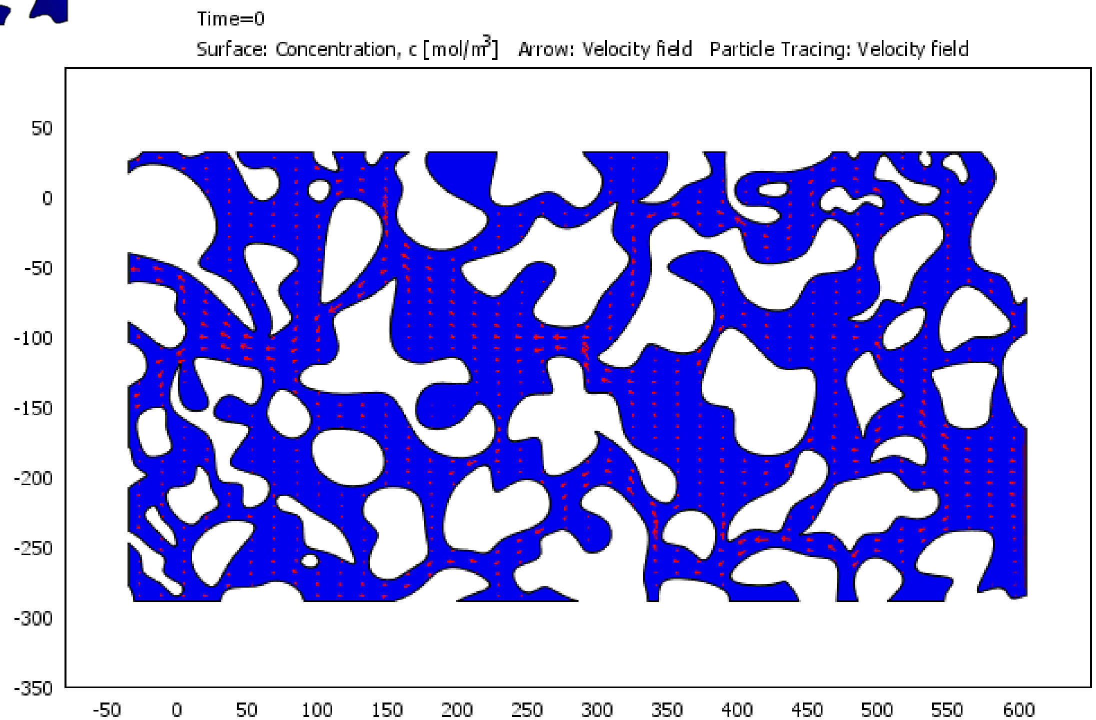
- · viscosity changes, mostly induced by temperature gradients
- · fluid density changes, induced by temperature or salinity gradients
-

Density changes are usually much smaller in their relative size than viscosity changes. However, in the vertical direction they effect the buoyancy, for which even small-size changes can have a significant impact.

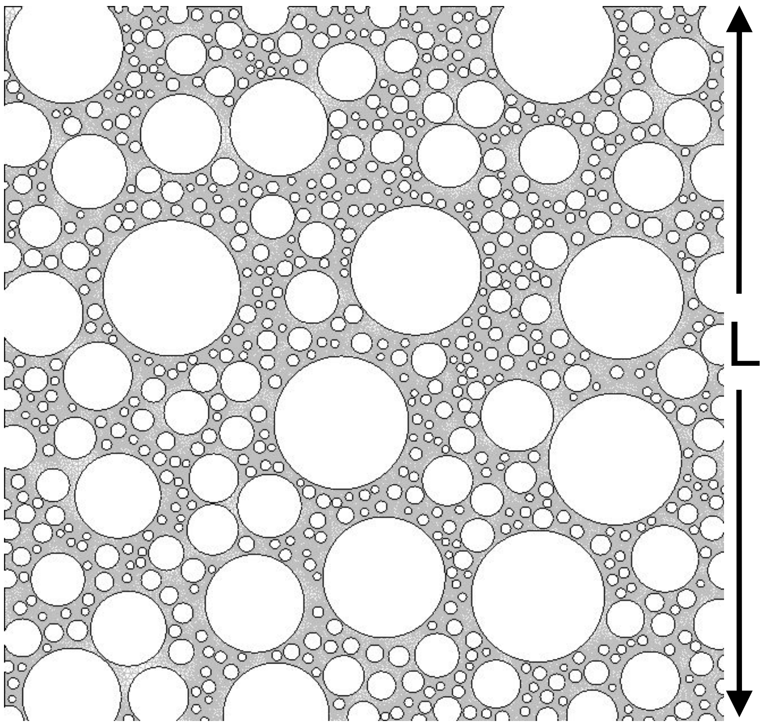
Concerning the flow we apply a pressure gradient from one side of the model domain to the other. The pressure difference thus scales linearly with L.

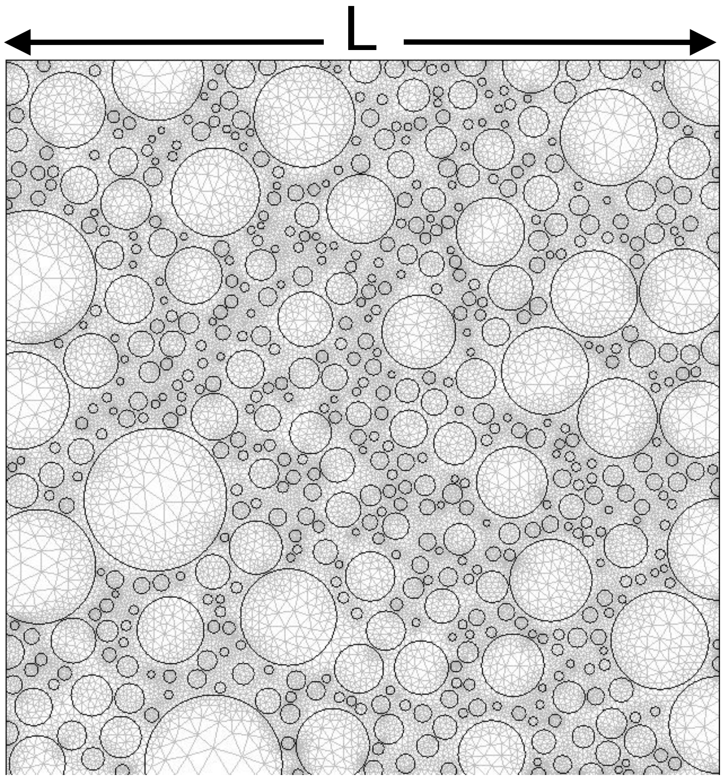
Pore-Scale COMSOL example





Artificial Porous Medium





Numerical experiments are performed in 2D artificial porous media. Using MATLAB® we construct a porous medium consisting of non-intersecting spheres of different size, using a random number generator for positions and diameters of the spheres.

Parameters

Parameter	*Value*	*Unit*
Molecular diffusivity	10^{-9}	m^2/s
Solid thermal diffusivity	$1.29\ 10^{-6}$	m^2/s
Fluid thermal diffusivity	$0.138\ 10^{-6}$	m^2/s
Mean velocity	$0.3\ 10^{-6}$	m/s
Porosity	0.8	1
Fluid density	1000	kg/m^3
Fluid viscosity	0.001	kg/m/s

Results: Flow

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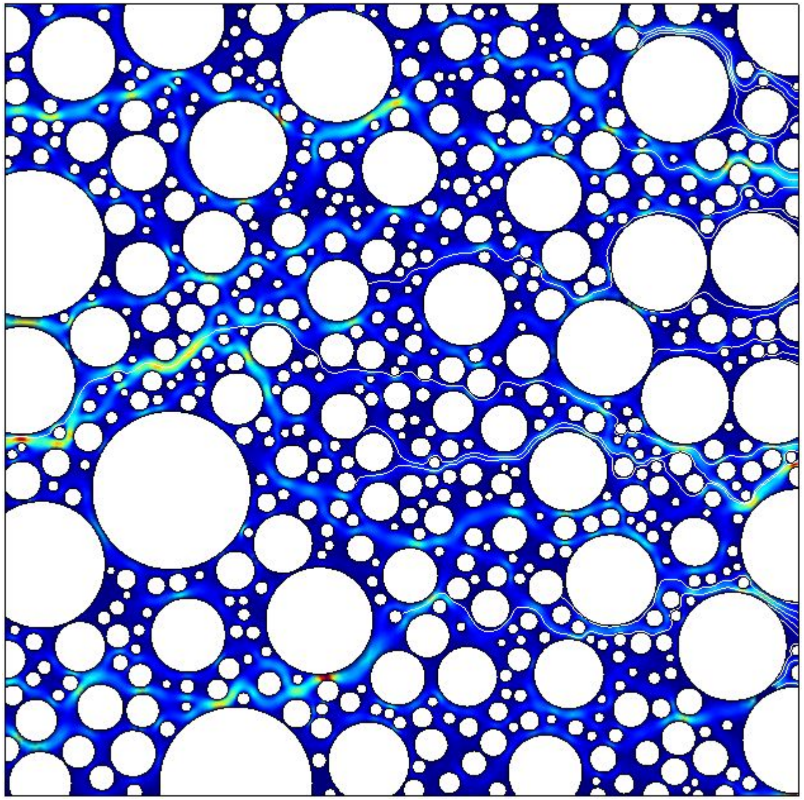
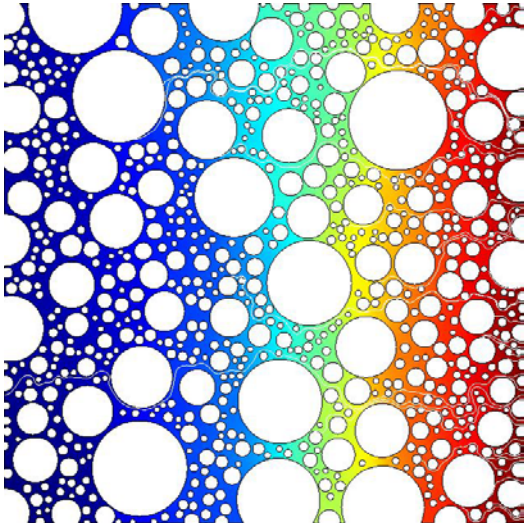
Typical flow field in an artificial porous medium; in color see velocity magnitude (red=high, blue=low), calculated solving Navier-Stokes equations in pore space

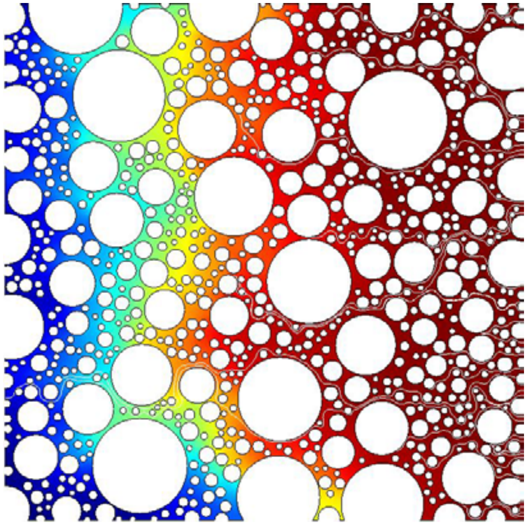


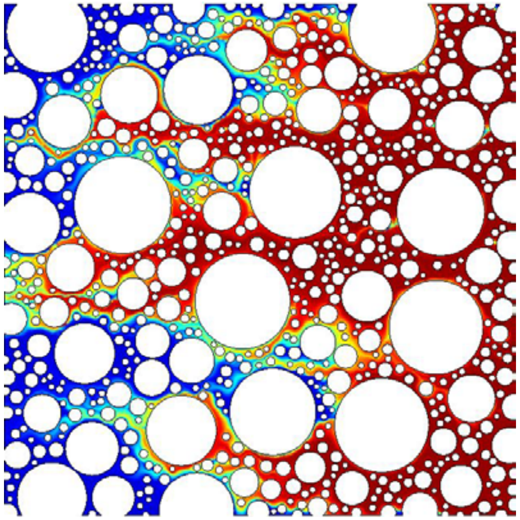
Results: Mass Transport



L = 1 mm,
T = 800 s

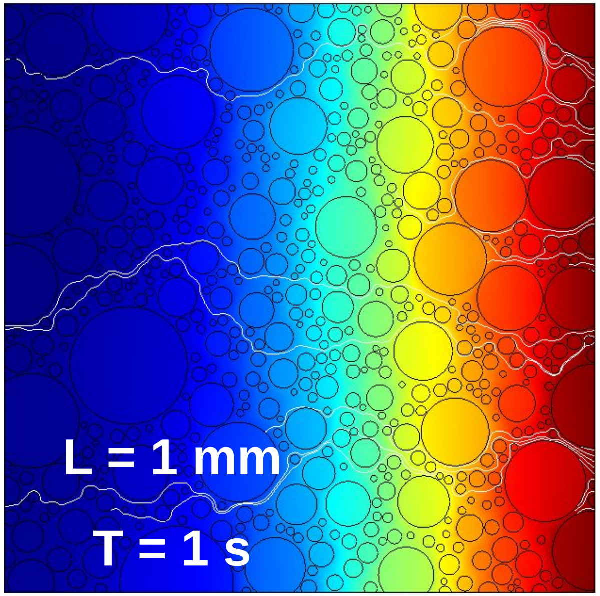
L = 10 mm,
T = 2000 s

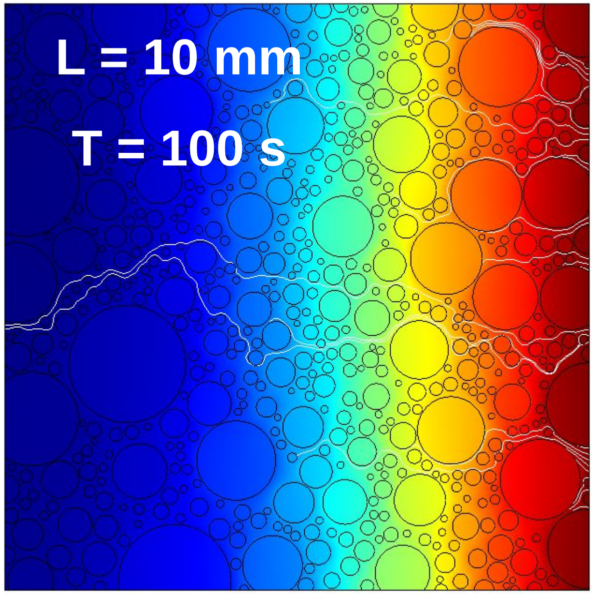


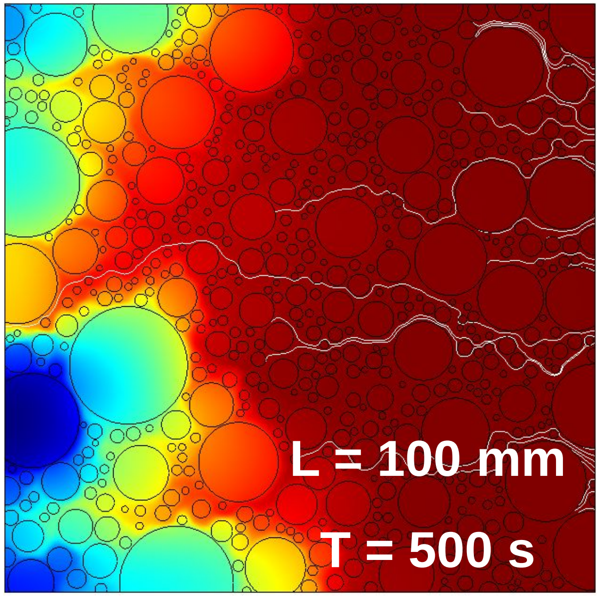


L = 100 mm,
T = 230 s

Results: Heat Transport







Discussion

- At the small scale, where diffusion dominates over advection, mass transfer can be understood as a highly retarded heat transfer

- At the intermediate scale mass diffusion is negligable against advection, while heat diffusion dominates over advection.

- Reason for the different phenomenolgy is the high Lewis number Le ≈ 1000 (ratio of thermal diffusivity / molecular diffusivity)
- Thus heat and mass transport can not be compared at that scale

- At the large scale, where mass diffusion processes are enchanced due to dispersion, heat transfer can be considered as a (slightly) retardated mass transport

Arrival Times

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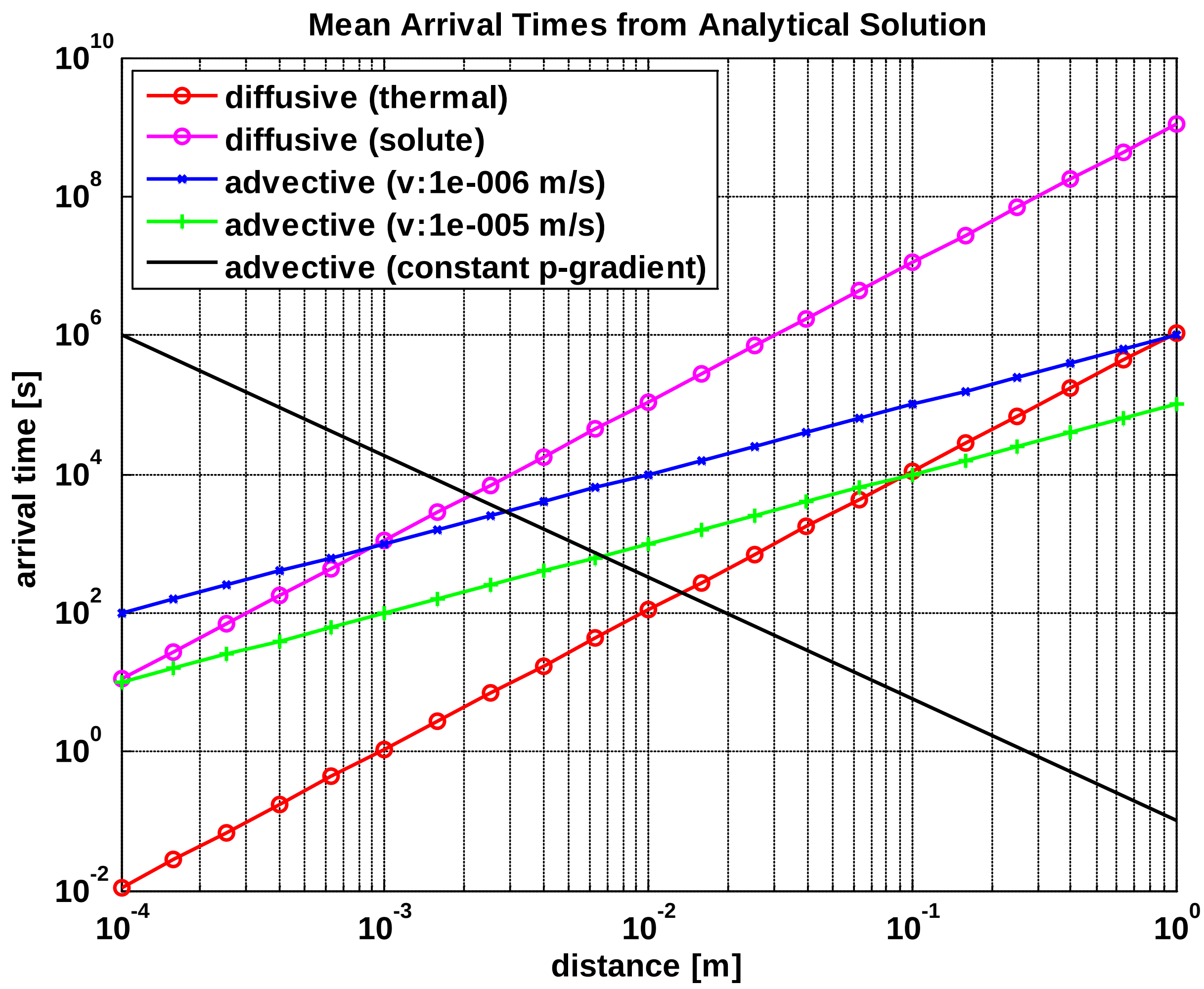

$$T_{diff} = \frac{L^2}{4D\left(erfc^{-1}\left(c/c_0\right)\right)^2}$$

$$T_{adv} = \frac{L}{v}$$

for constant p-gradient: $v \sim L^2$

Conclusions

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As a result of the modelling work we find a strong scale dependence.

- At the microscale (<1 mm) heat and mass transport are both diffusion dominated and the differences are determined by the highly unequal diffusivities

- At the large scale (> 1m) heat and mass transfer are advection dominated; heat is retarded

- At the intermediate scale (>1 mm, < 1m) heat transfer is diffusion dominated, while mass transfer is advection dominated; thus incomparable

Reference & Acknowledgement

Holzbecher, E., 2012. Environmental Modeling – using MATLAB, Springer Publ., Berlin/Heidelberg, 2nd Ed.

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