Supplementary of “Experimental investigation of the interplay between transverse mixing and pH reaction in porous media”

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1 Simulating the tracer and reactive experiments

The 2D tracer and pH experiment results in 3.1 and 3.2 respectively (and for convenience, are presented again in figure S1.1, and S1.2. respectively), were reproduced using a COMSOL Multiphysics simulator (figure S1.3. and S1.4. respectively). This was done by importing the cell AutoCAD design to COMSOL so an exact Stokes flow simulation could be employed to solve the flow field. The same parameters for the diffusion of the R6G and Darcy velocity were taken, and a forward solver was used to calculate the transverse dispersion.

The simulation reproduced the initial invasion scheme for the experimental setup, and as in the experiment, the steady state was verified by comparing the output of consecutive time frames in the simulation. Comparing Figure S1.1. with Figure S1.3. shows that the simulation captures well the transverse dispersion for all Pe values, although it will enhance the dispersion for the low concentrations.

As in the tracer experiment, we use the same Stokes flow solver for the reactive experiment and update the diffusion coefficient to the higher value of the OH^-, and the H^+ migration, providing the pH value based on both ion and proton diffusion. As the pyranine emission intensity range is given by equation 5, as shown by the exponential decay in Figure 2.b., a similar exponential conversion was used in the COMSOL simulation to highlight this region. Comparing the experimental and simulated reactive case (Figure S1.2. and Figure S1.4, respectively), show that the high Pe simulation produced similar results to the experimental values, yet the low Pe values proved more challenging. This difference between the simulation and experimental results, even when considering the pH exponential range, did not improve when we considered the Nernest-Planck equation. We believe that the discrepancy stems from the fact that while diffusion is indeed higher, the neutralization reaction of the OH^- ions, and H^+ proton, following their local concentration, requires a model that also considers both the diffusion and local concentrations. Another aspect that is not considered in the COMSOL model is the Grotthuss mechanism and the strong polarization power leading to the immediate binding to an intact water molecule to form hydronium ions by creating covalent bonds. This mismatch between the model and the experimental setup clearly points to the need to incorporate these mechanisms in existing models.

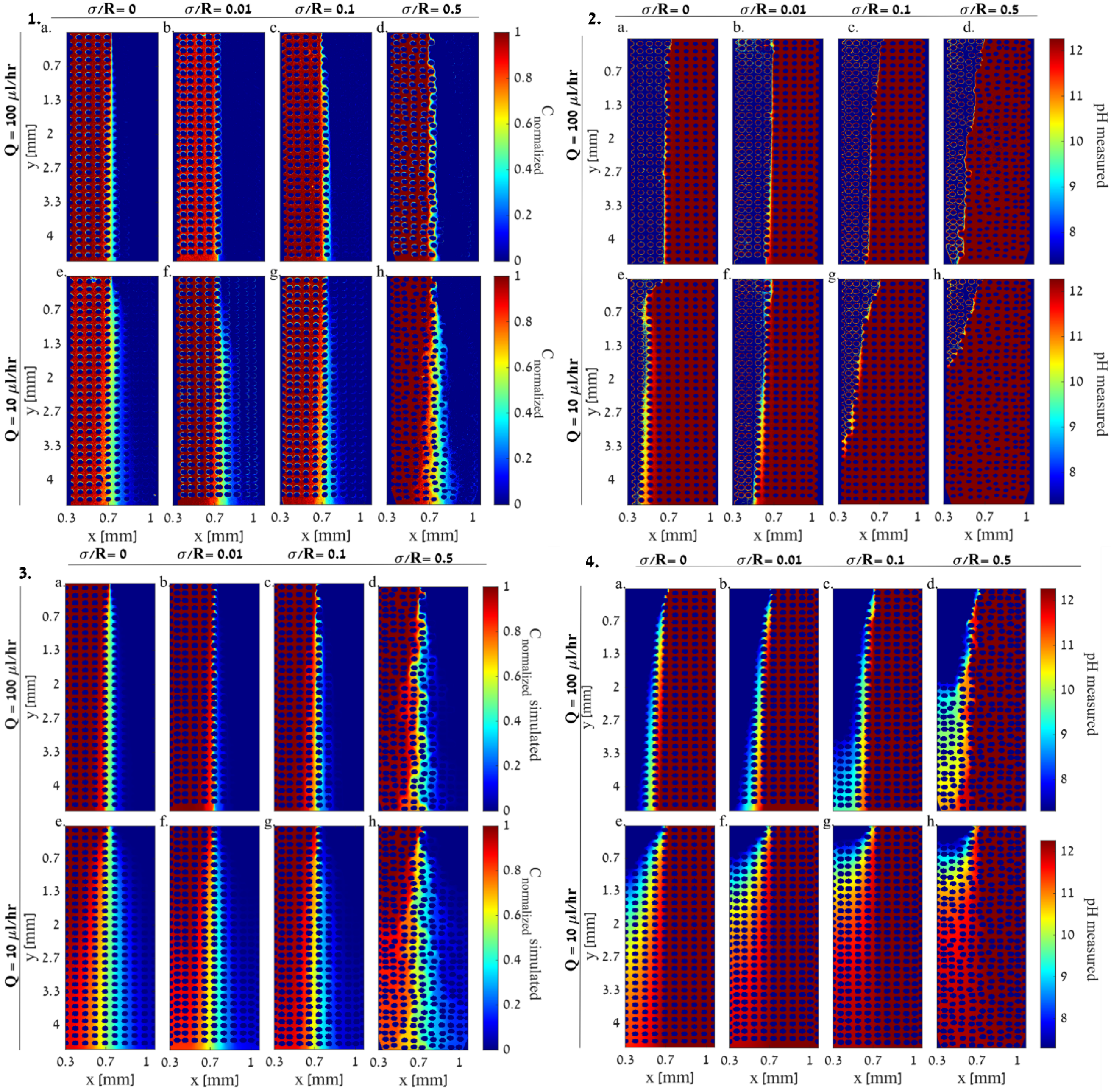

Figure S1.1. Mixing experiments: distribution of the conservative tracer normalized concentration. a.-d. Flow rate of 100 µl/hr at medium heterogeneities of of σ/R=0, σ/R =0.01, σ/R =0.1 and σ/R =0.5, respectively. e.-h. Flow rate of 10 µl/hr at medium heterogeneities of of σ/R=0, σ/R =0.01, σ/R =0.1 and σ/R =0.5, respectively. 2. Reactive experiments: pH values as indicated by the reactive tracer distribution for similar conditions. 3. Simulated mixing experiments distribution of the conservative tracer simulated by COMSOL for similar conditions. 4. Simulated reactive experiments: pH values simulated by COMSOL for similar conditions.