

# Chemical reactions under flow heterogeneities

Lazaro J. Perez, IDAEA-CSIC,  
Juan J. Hidalgo, IDAEA-CSIC,  
Marco Dentz, IDAEA-CSIC

**Key words:** reactive transport, mixing, reactive random walk particle tracking

## Abstract

Evaluation of the mixing process in aquifers is of primary importance when assessing attenuation of pollutants. Fluid mixing controls chemical reactions that are fast compared to mass transfer processes. Chemical reactions are local phenomena that fluctuate at the pore scale but predictions are often made at much larger scales. Aquifers exhibit heterogeneities at all scales which generate flow variabilities that creates complex concentration distributions that enhances or reduce mixing and thus chemical reactions. Determination of the impact of flow variability at pore scale is key to understand the behavior of mixing-driven chemical reactions.

We study a bimolecular irreversible chemical reaction  $A + B \rightarrow C$  in a laminar Poiseuille flow reactor to analyse and quantify the impacts of flow heterogeneity in a single pore. We use a reactive random walk particle tracking method which represents the reactants by particles. We observe three different time regimes characterized by different behaviours of the product formation (see Figure 1). Mixing is dominated by diffusion at times smaller than the advective time ( $\tau_V$ ), time in which the solute covers the same distance by diffusion and by advective transport with the mean flow velocity. For times larger than  $\tau_V$ , where advection inhomogeneity begins to dominate over diffusion, we find enhanced reaction efficiency due to flow variability. Finally, for times larger than the characteristic time of diffusion ( $\tau_D$ ), we find that mixing is represented by the Taylor dispersion coefficient. We characterize mixing in the reaction by introducing the dispersive lamella model, based on the effective dispersion coefficient, which captures the features of stretching, compression and coalescence of the mixing front in the reaction and accurately predicts the total mass of product C. We compare our effective model prediction of product mass to other predictions using traditional approaches such as the apparent dispersion coefficient, and the stretched lamellae theory which measures mixing through diffusive flux in a stretching interface (see Figure 1). We find that our effective model is able to describe the impact of flow heterogeneity on mixing-driven reactions at pore scale. By contrast, the use of the apparent dispersion coefficient, or the stretched lamellae theory overestimate the width of the mixing zone, and thus the chemical reaction, when flow heterogeneity dominates over diffusion.

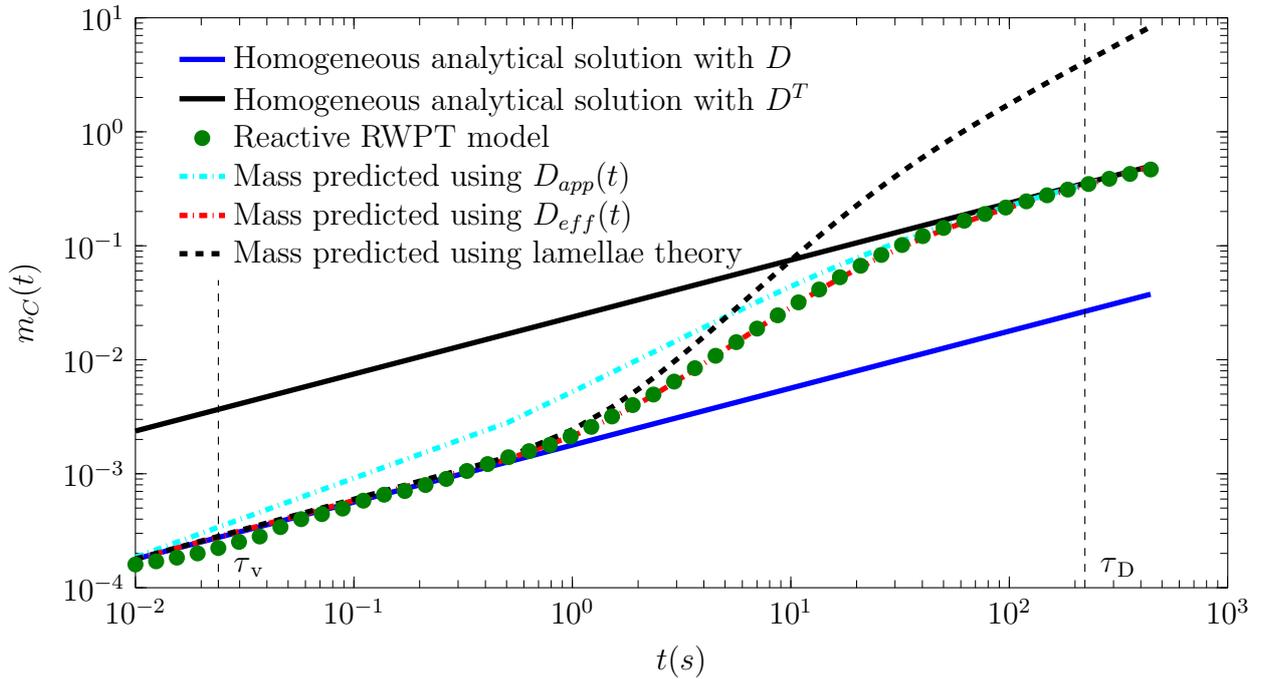


Figure 1: Total mass of product C formed in the chemical reaction. Homogeneous analytical models coupled with diffusion ( $D$ ) and Taylor dispersion coefficient ( $D^T$ ) can predict the total mass production at early ( $t < \tau_V$ ) and late ( $t > \tau_D$ ) times respectively. The lamellae theory and apparent dispersion coefficient ( $D_{app}(t)$ ) predictions agree the simulation results at early times, however both approaches overpredict the reaction at intermediate times ( $\tau_V < t < \tau_D$ ). While only the effective dispersion coefficient ( $D_{eff}(t)$ ) prediction reproduce the simulation results at all times. At late times,  $D_{app}(t)$  and  $D_{eff}(t)$  predictions match, while the lamellae theory overestimates the reaction.