



Effects of advection and reaction rates on pattern formation in replacement reactions

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Replacement reactions during fluid infiltration into porous media, rocks and buildings are known to have important implications for reservoir development, ore formation as well as weathering. Natural observations and experiments have shown that reaction fronts in these processes can appear very differently with sharp fronts on the one hand opposed by rough fronts with fingers and grain boundary or fracture dominated reactions on the other hand. Most observations are based on the actual reactions, which are then used to predict how the material was transported into the system. However, it is not clear how reliable this approach is and what the reaction patterns actually tell us about the processes involved. In this contribution we show a first approach to model experiments of replacement reactions in grain aggregates with permeable grain boundaries testing systematically the effect of variable advection, diffusion and reaction rates on reaction front evolution. In the numerical models that are run in the software Elle, fluid percolates through a square block constituted by a grain aggregate. Fluid infiltrates from all block boundaries with concentration advecting and diffusing into the system from these boundaries. Reactions occur if the local concentration is sufficiently high, at the same time the concentration change in the entire system (both fluid and solid) is monitored continuously. Results show that sharp fronts are formed when either diffusion is dominating or the reaction is very fast. Roughness develops when advection is dominating and the reaction is relatively slow. Extreme roughness across several grains and even the whole aggregate develops when advection is moderate to high and the reaction is slow. In non-dimensional phase space using Peclet and Damkohler numbers smooth fronts form at low Peclet and high Damkohler numbers, whereas roughness forms at high Peclet and low Damkohler numbers. The smooth to rough transition is sharp on the low Peclet side where diffusion becomes dominant but has a slope towards higher Peclet numbers. The latter results in fronts at constant Damkohler numbers that are first smooth at low Peclet numbers, then become rough once advection is becoming important and then become smooth again because reaction rates take over. Our results indicate that reaction rates are crucial for the formation of patterns, and that the shape of reaction fronts is only partly due to the underlying transport mechanism of material.