

# **A Brief History of Reactive Transport--The Early Days**

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The first major milestone in the history of reactive transport was a work that did not explicitly include transport at all, but represented the first geochemical thermodynamic model that considered irreversible processes: Helgeson's 1968 and 1969 papers on "Evaluation of irreversible reactions in geochemical processes involving minerals and aqueous solutions". By considering irreversible processes for the first time, Helgeson opened the scientific floodgates and various papers specifically including transport processes followed relatively quickly. These include Peter Lichtner's landmark paper in 1985 in *GCA* that laid out rigorously the basis for a continuum approach to multicomponent reactive transport. And shortly following, his paper on the Quasi-Stationary approach (1988) that generalized the reaction path model for transport by introducing a Lagrangian fluid packet migrating the reactive rock or sediment. In 1989 George Yeh and Tripathi published what I would say was the first general "environmental reactive transport" code in multiple dimensions, driving the first (of many) wooden stakes into the heart of the constant linear distribution coefficient ( $K_d$ ) model for chemical reaction. Steefel and Lasaga (1994) presented a reactive flow and transport model for non-isothermal, kinetically controlled water-rock interaction and fracture sealing in hydrothermal systems. This study was the first to consider multicomponent reactive transport in the context of non-isothermal flow fields, and was also apparently the first to consider how reaction-induced permeability change (clogging) could alter the flow field in such systems. Published over the objections of two prominent hydrologists, this study was followed closely by another authored by Steefel and Lichtner (1994) who presented the first diffusion-reaction model with a kinetic treatment of reactions, combined again with model predictions of porosity (and transport) change that were verified later by isotope geochemistry. In a very different environment, Van Cappellen and Wang (1996) and Wang and Van Cappellen (1996) showed that most of the  $O_2$  in shallow marine sediments was actually consumed in reactions with  $H_2S$  diffusing from the sulfate reduction zone at depth, and not due purely to aerobic respiration. This result, which apparently was not widely recognized at the time, emerged very naturally from the multicomponent reactive transport modeling.