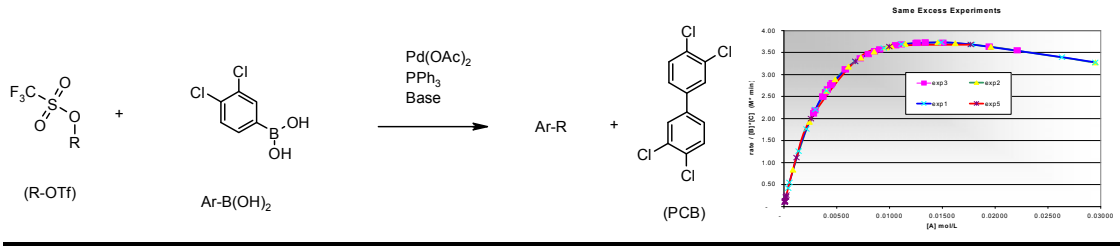

Cross coupling of unsaturated aryl or vinyl triflates/halides with aryl boronic acids using Pd as catalyst (Suzuki coupling) have become increasingly attractive for making the hetro-coupled product (Ar-Ar'). However, most Pd cycle reactions produce some homo-coupled impurity. This is a major concern when the impurities are Polychlorobiphenyl's (PCBs). To understand and control the impurity formation was the most important challenge. This paper demonstrates how reaction progress analysis along with mathematical modeling can be used to gain fundamental understanding and postulate reaction mechanism, thereby provide an insight on how to reduce the amount of by-product generated in catalytic cycle with limited number of experiments (typically three). Fundamental such as, stability of catalyst, catalyst poisoning, inhibition, reaction mechanism can also be answered with these limited number of experiments. Characterization of the catalytic cycle led to a semi-batch addition regime of boronic acid, which effectively eliminated PCB generation by forcing the catalytic cycle to partition between the oxidative addition intermediate (I) and transmetallated intermediate (III).