# Reaction building for chemical and biochemical systems

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Modeling of chemical and biochemical systems is often necessary in order to predict conditions which give the optimal yields in reactors. However, in most cases models are required for systems where the exact reaction mechanism is unknown. So the first step in model building should be the construction of a reaction network containing all the relevant reaction steps which are happening.
Starting from information including the knowledge of raw materials, products, byproducts and any known intermediates we have developed methodology for the prediction of reaction networks containing all possible reaction steps. For biochemical systems an alternative method is developed based on the enzymes present which catalyze and enhance the reactions.
Furthermore, kinetic models are generated by fitting suitable kinetic expressions for each reaction step using experimental data. Based on the fitting results we find that it is usually not necessary to include all of the predicted reaction steps and simpler models can be obtained for use in reactor design and optimization.