Model formulation and interpretation
for chemical reactions mechanisms
- from experiment to theory

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From kinetics study of a given pair of reactants different types of mechanisms were investigated. A mathematical model was formulated. Model parameters were evaluated and assessed. Obtained results from the optimization procedure opened an interesting discussion about the limits of parameters obtained from experiments data for imposed conditions, such as mechanism type and collecting procedure.

By using of a least squares method, obtained models as best fits correlates with experimental measurements; the results shown an average of 96.6% for a sample size average of 2967 pairs of data.

Comparing the results obtained by different experiments, all obtained parameters, which were not related with the experimental conditions, were in same range of 95% confidence interval. These results validates experimental data and as well as data obtained by model.