Let us first define a atom set ,

In which represents “hypothesized atom”. Then define the species set ,

For example, to the n-propane combustion mechanism at low temperature (650K-900K),

shall have a number of distinct subsets. But not all the subsets out of is of chemical kinetic interest. Naturally one can choose to study subsets to which all elements contain the same atom, such as O atom, H atom or He atom etc. For example, one can study subsets like

Notice , and differ from one another in the number of Oxygen atom each element can have. In other words, the type of atom and the number of atom are both important when choosing subsets to study. We find it to be convenient to define “species-atom-composition” set ,

For example, to the n-propane combustion, one subset of is

is equivalent to the natural composition of species. One can define “species-atom-composition” using the “hypothesized atom”. For example

The “species-atom-composition” is important for the following reasons,

1. It automatically selects species of interest. In other words, it is naturally equivalent to a subgraph and helps to construct subgraph.
2. It helps to calculate branching ratio. “c” in triplet (s, a, c) represents number of atom “a” species “c” contains, one needs this information to calculate branching ratios when evaluating pathway probability.

Use as an example, one can use to construct a subgraph,

From this subgraph, at least three important pathways can be extracted,



From a static point of view, pathway 3 should contain pathway 1 and pathway 2. It is not true in our time-dependent pathway representation because of the survival probability of and . and can stay as and and do not react, therefor don’t produce OH radical. Simply, the effect number of OH that one OH can diverts into should be