First of all, the carbon subgraph is used. One single fictional atom, namely “HA” is hypothesized to be inside all species from carbon subgraph. For example, to , instead of having 3 carbon atoms, it is assumed that has one single “HA”. The new species composition dictionary is like in Table 1,

Table . Hypothesized atom composition of species from carbon subgraph

|  |  |  |
| --- | --- | --- |
| Species name | Carbon | HA |
|  | 3 | 1 |
|  | 3 | 1 |
|  | 3 | 1 |
|  | 3 | 1 |
|  | 3 | 1 |
|  | 3 | 1 |
|  | 1 | 1 |
|  |  |  |

The reaction network is constructed in the conventional way, that treating species as vertices, all possible reactions as edges. Since the tagged atom now becomes a hypothesized “HA”, when it comes to generate pathway and evaluate pathway probability, “HA” is presumably be followed. For example to the top 3 most probably pathways from time 0 to time 0.9, (ignition delay time, has a value of 0.78s in n-propane combustion mechanism with K, =10 bar, =1) as below,

The pathway probabilities and number of net OH being produced along each pathway is summarized as in Table 2 below,

Table . Pathway probabilities and net number of OH being produced along top 3 most probable pathways

|  |  |  |
| --- | --- | --- |
|  | Pathway probability | Net OH produced |
| Path 1 | 0.20 | 3 |
| Path 2 | 0.14 | 1 |
| Path 3 | 0.13 | 0 |

Then the Merchant f value, using top 3 pathway, is simply calculated as

Instead of using top 3 pathways, larger number of pathways can be used. I actually top 100 most probable pathways to calculate the Merchant f value. Beyond time 0.9, f value at more time points was calculated.

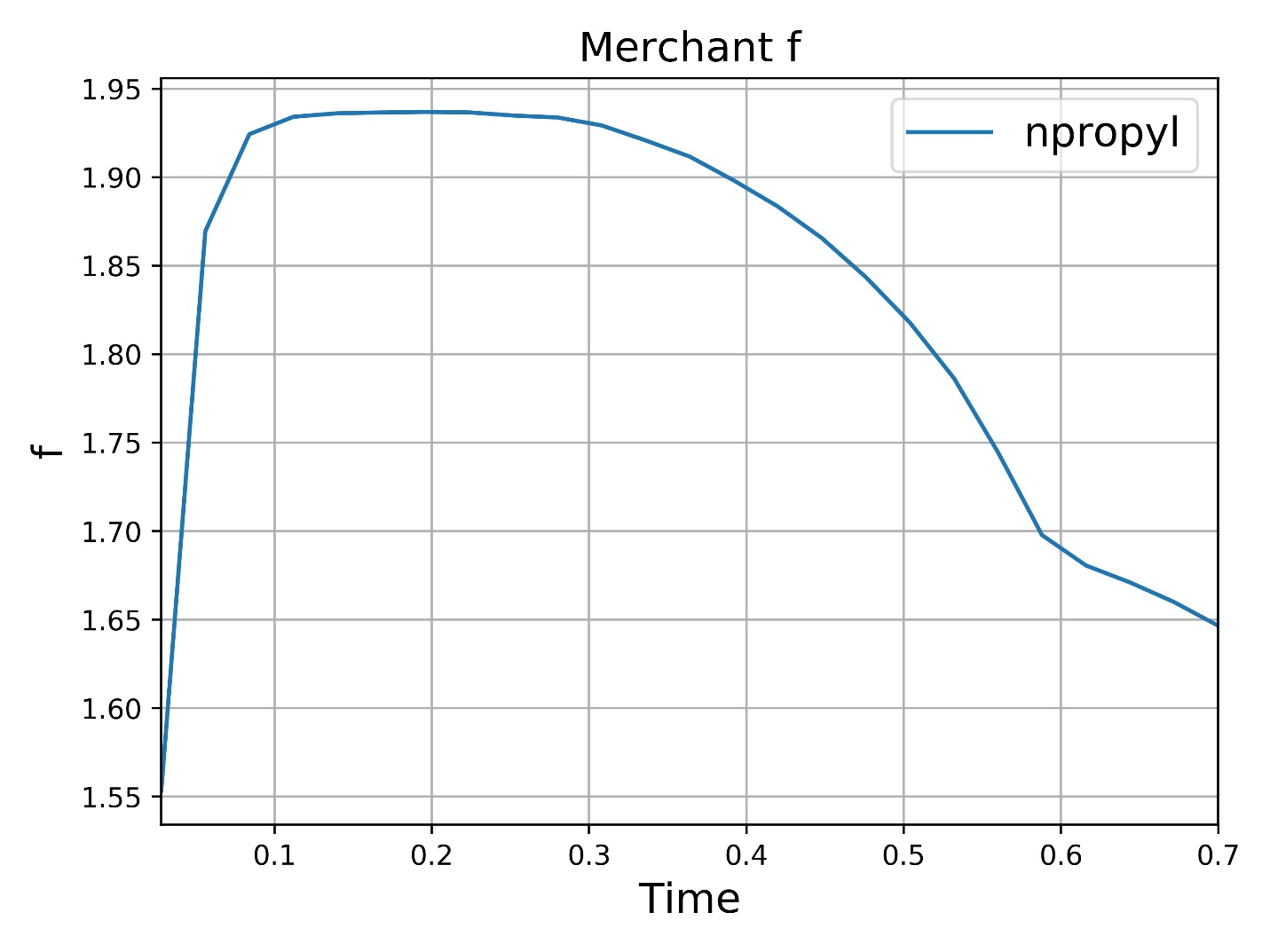


Figure . Merchant f value of n-propyl subgraph

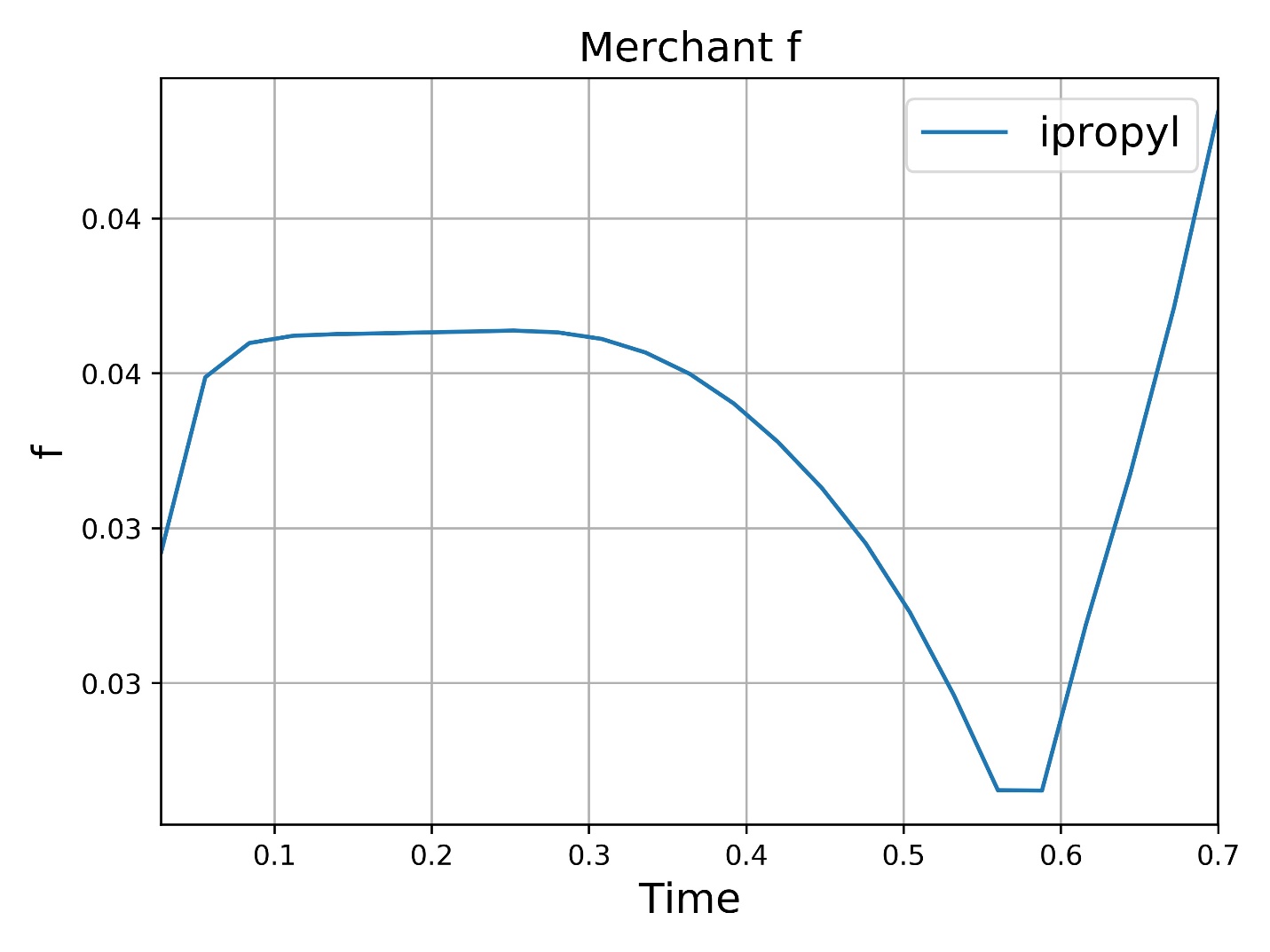


Figure . Merchant f value of i-propyl subgraph

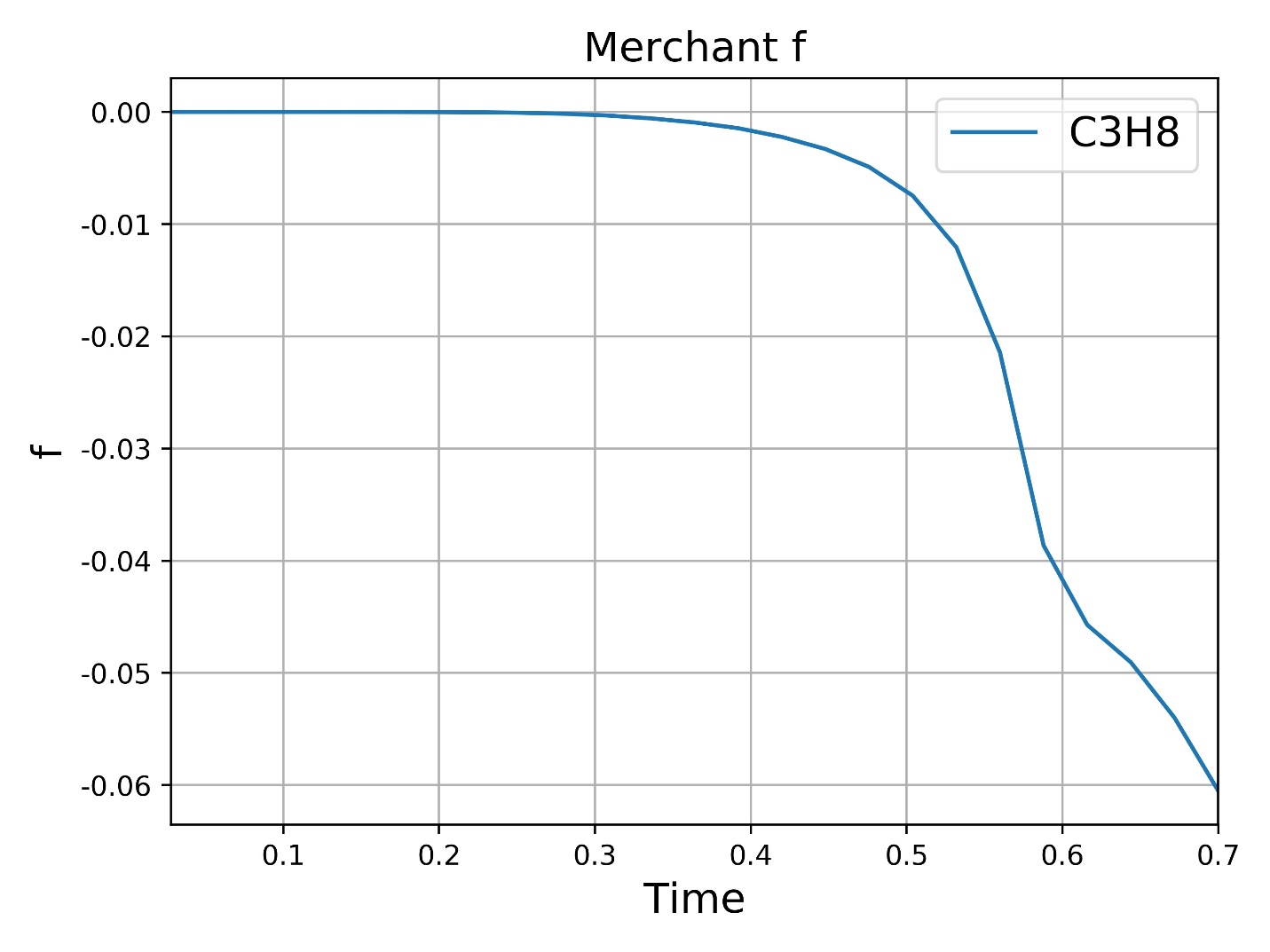


Figure . Merchant f value of n-propane subgraph