Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

ReacNetGenerator: An Automatic Reaction Network Generator for Reactive Molecular Dynamic Simulations

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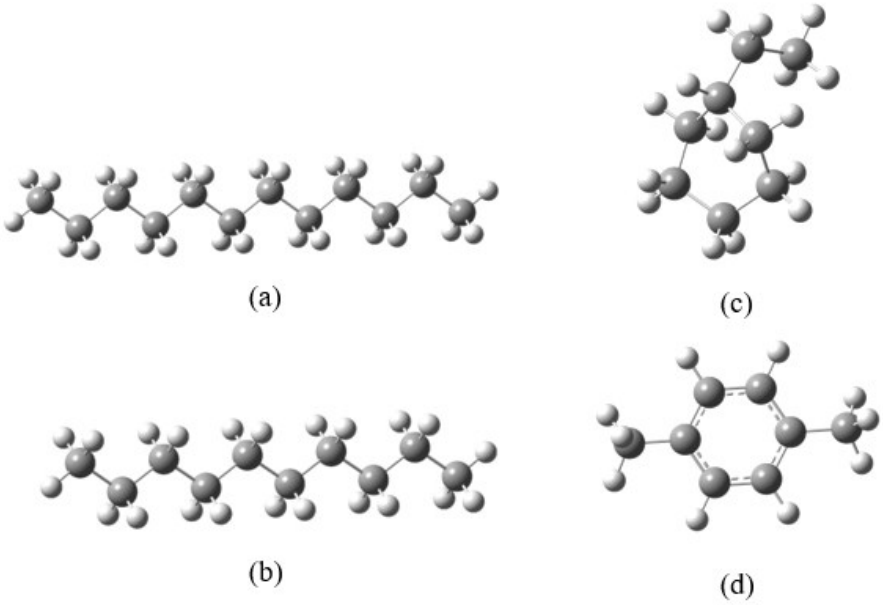

Figure S1. The 4-component RP-3 contains (a), 42% *n*-dodecane (*n*-$C_{12}H_{26}$), (b), 40% *n*-decane (*n*-$C_{10}H_{22}$), (c), 13% ethylcyclohexane (C_8H_{16}), and (d), 5 % *p*-xylene (C_8H_{10}).

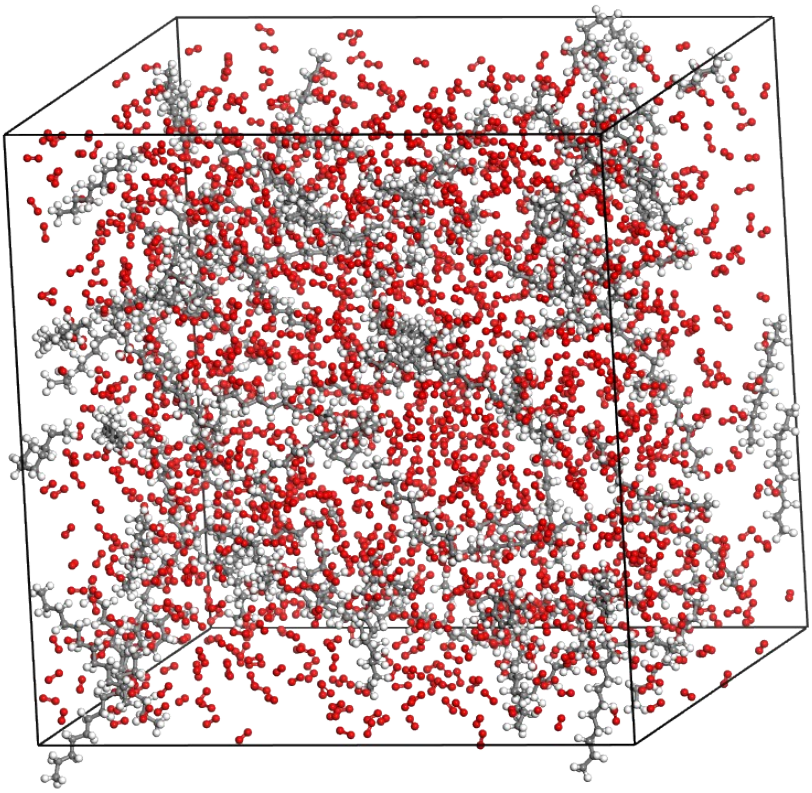

Figure S2. Starting configuration of RP-3 combustion system (6490 atoms). The gray balls represent C, white represent H, and red represent O, respectively.

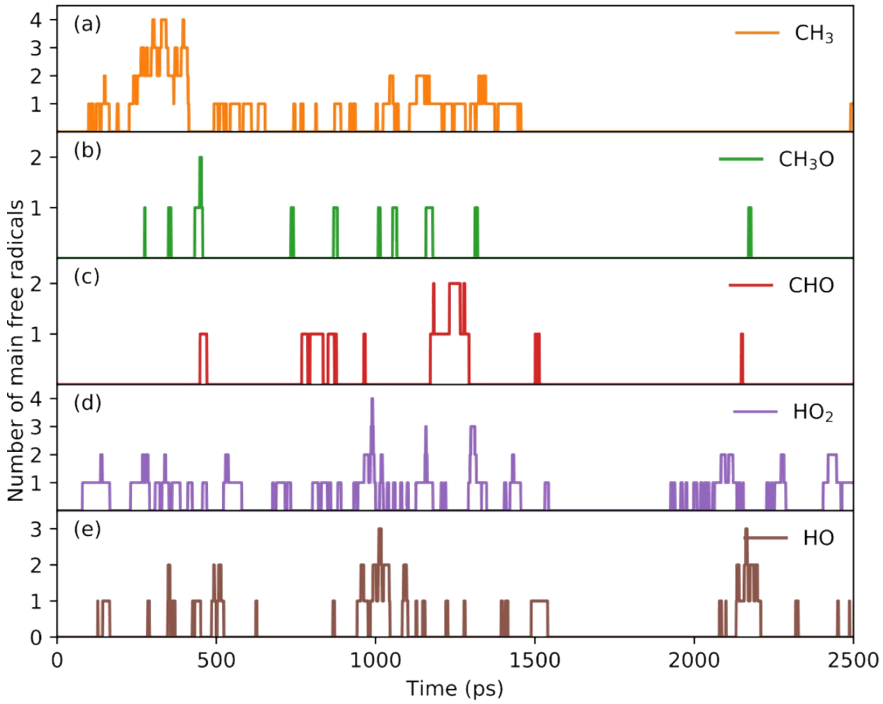

Figure S3. The number of important intermediates evolved with simulation time.

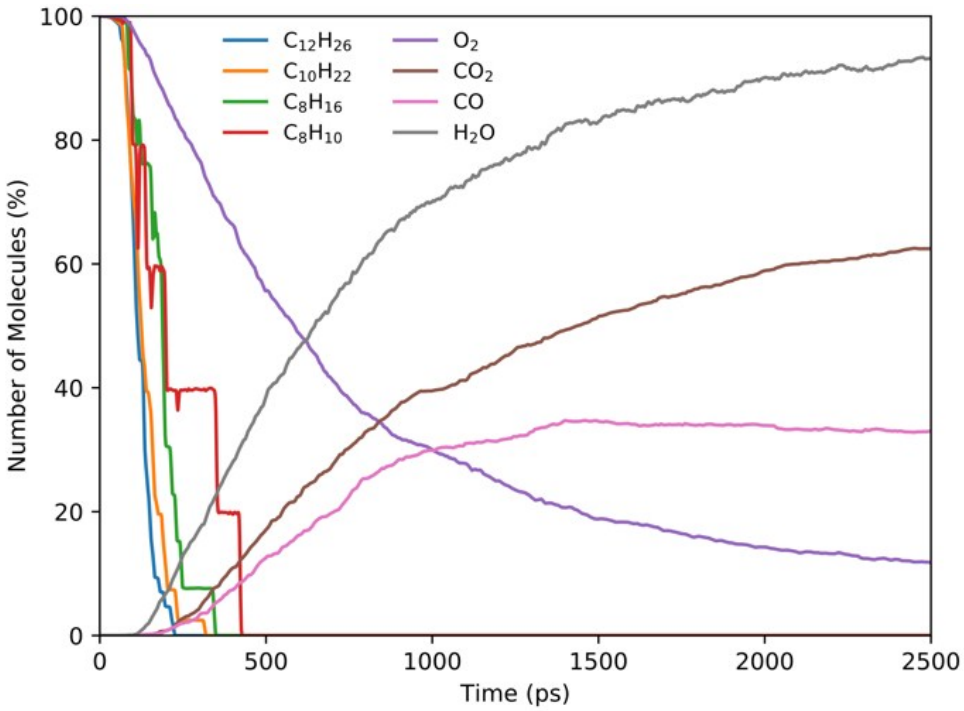

Figure S4. The distribution of reactants and products during the MD simulation.

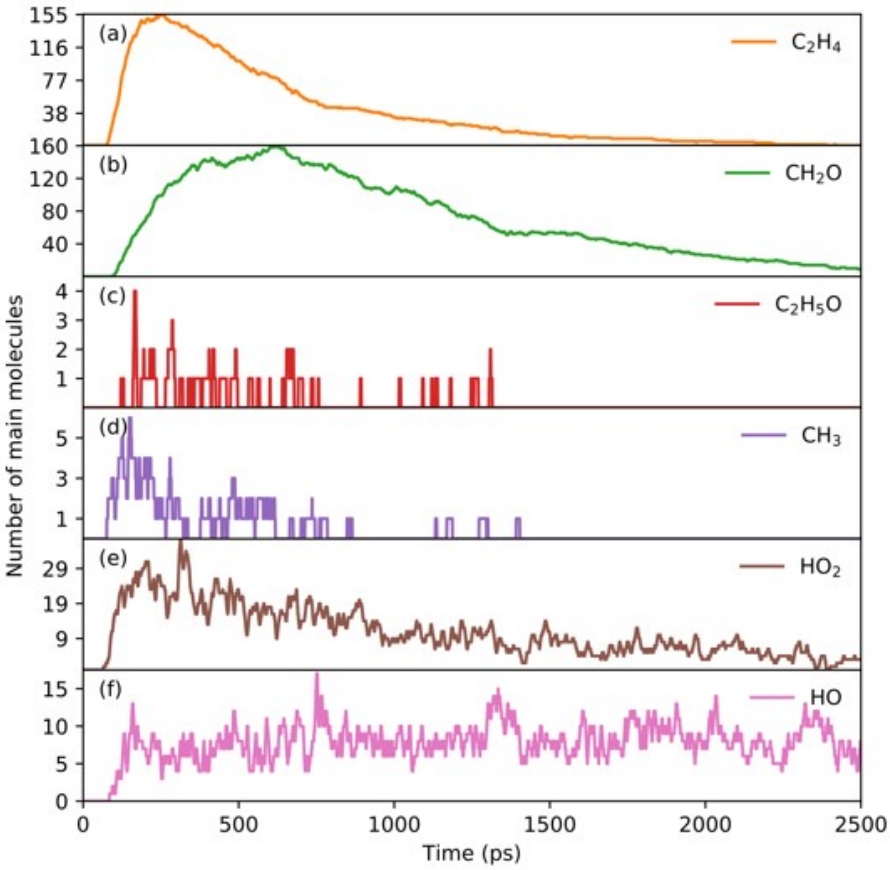

Figure S5. Distributions of important intermediates and radicals during the MD simulation.