Supplementary Information (SI) for RSC Advances.
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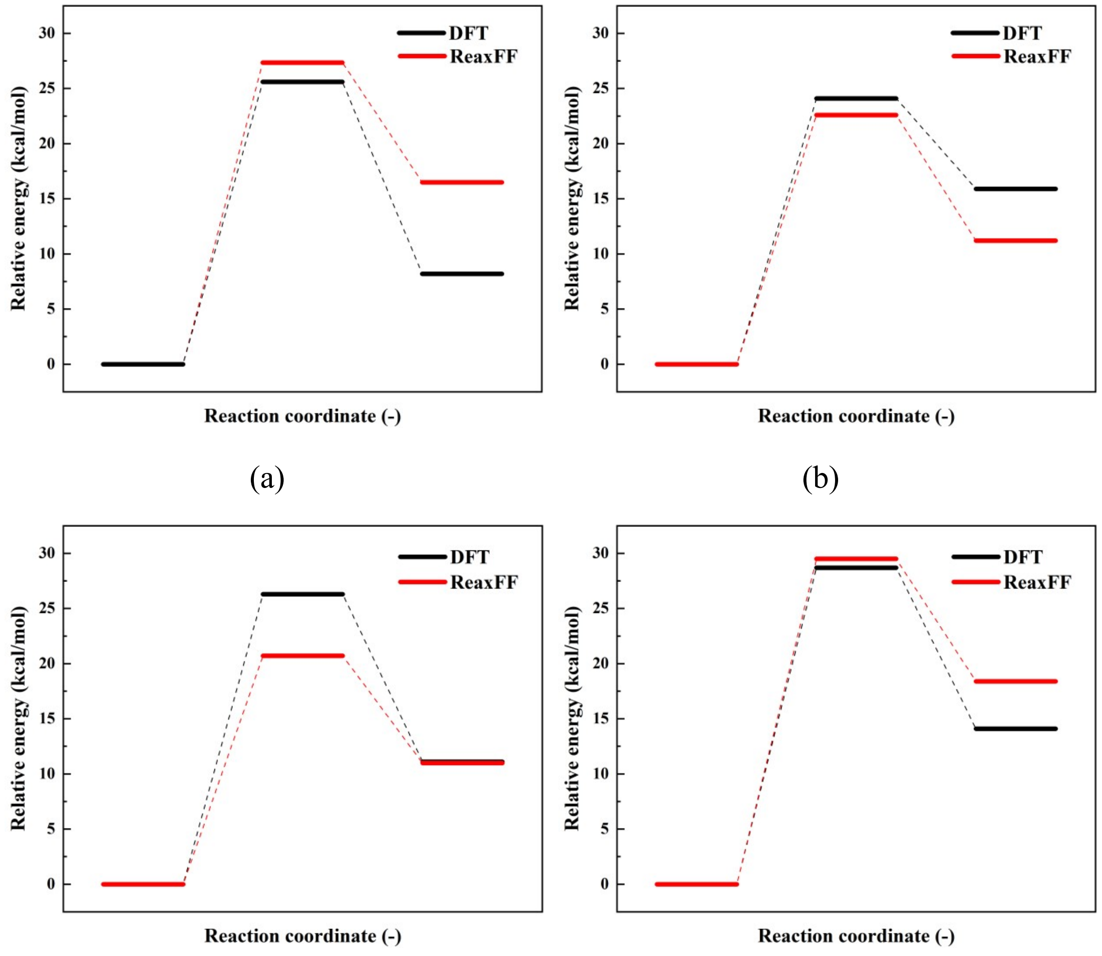
Supplementary Materials

We conducted a systematic assessment of the employed ReaxFF force field from two perspectives: reaction energy barriers and thermal stability.

First, as shown in Fig. S1, four representative ring-opening reaction pathways involved in the thermal decomposition of JP-10 were selected, corresponding to the R1, R2, R3, and R6 reaction channels defined in Yue et al.[1]. For identical reaction configurations, the reaction energy profiles predicted by the present ReaxFF force field were compared directly with density functional theory (DFT) results reported in Yue et al.[1]. The comparison shows that ReaxFF reproduces both the activation barrier heights and the overall trends in relative energy variations with agreement to DFT. These results indicate that the employed ReaxFF force field is capable of reasonably capturing the key energetic characteristics of the initial bond-breaking processes in JP-10 pyrolysis, thereby providing a reliable basis for describing the reaction kinetics of JP-10-containing systems.



(a) (b)

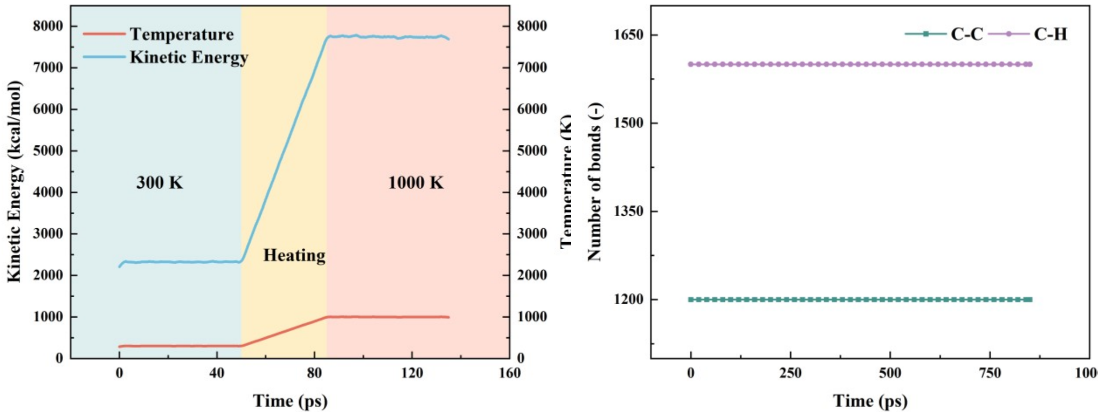
(c) (d)

Fig. S1. Relative energy profiles of the major ring-opening reaction pathways of JP-10 predicted by DFT and ReaxFF: (a) R1; (b) R2; (c) R3; (d) R6.

Furthermore, to verify the stability and kinetic soundness of the ReaxFF force field in multi-molecular JP-10 systems, molecular dynamics simulations were performed to examine the behavior of a pure JP-10 system under heating and elevated-temperature conditions. Previous studies have demonstrated that JP-10 exhibits good thermal stability below 1000 K[2]; therefore, 1000 K was selected as the target temperature for force-field stability validation in this work.

Specifically, a system containing 100 JP-10 molecules was constructed, with an initial density of 0.94 $g\cdot cm^{-3}$ and a simulation box size of 28.9 Å × 28.9 Å × 28.9 Å. The system was first equilibrated at 300 K for 50 ps, followed by a linear temperature ramp from 300 K to 1000 K over 35 ps. Subsequently, the system was further evolved at 1000 K for an additional 50 ps. During the simulations, the temporal evolution of system temperature, kinetic energy, and the number of major chemical bonds (C-C and C-H) was monitored.

As shown in Fig. S2, both the temperature and kinetic energy remain stable throughout the heating and isothermal stages, with no evidence of nonphysical energy drift. Meanwhile, the numbers of C-C and C-H bonds remain essentially constant at 1000 K, and no noticeable thermal decomposition is observed. These results indicate that the employed ReaxFF force field not only provides a stable description of the reactivity of isolated JP-10 molecules, but also correctly reproduces the thermal stability characteristics of JP-10 in multi-molecular systems under moderately high-temperature conditions.



(a) (b)

Fig. S2. Thermal stability of the multi-molecule JP-10 system described by ReaxFF: (a) evolution of temperature and kinetic energy during equilibration, heating, and isothermal stages; (b) temporal evolution of the numbers of C-C and C-H bonds at 1000 K.

References

1 L. Yue, H. Xie, X. Qin, X. Lu and W. Fang, *J. Mol. Model.*, 2013, **19**, 5355-5365.
2 H. Liu, J. Liang, R. He, X. Li, M. Zheng, C. Ren, G. An, X. Xu and Z. Zheng, *Combust. Flame*, 2022, **237**, 111865.