Soot nanoparticles decomposition: Molecular dynamics and Monte-Carlo modeling

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Carbon soot sublimation temperature varies in a wide range from 2000 to almost 4500 K depending on formation conditions in the flame [1, 2]. Such differences in sublimation temperatures can be caused by variations in morphology and different contributions of non-covalent interactions and chemical bonding in the stability of carbon nanoclusters. In order to estimate soot sublimation temperature and to shed the light on molecular products of decomposition in this work we model high temperature carbon nanoparticle decomposition by various approaches: algorithmic clustering, Monte-Carlo cutting simulation and molecular dynamics simulation. Reax force field is selected for MD modeling of soot fragmentation. And for Monte-Carlo simulation a self-developed divisive algorithm is used. All approaches show similar results in the size distribution of decomposition products which proves correctness of used methods. High decomposition temperature results in low molecular ($C_2 - C_3$) products and under lower temperature soot breaks into graphene-like products with molecular weight in range 200-600 Da.

[1] Eremin A V, Gurentsov E V, Kolotushkin R N and Mikheyeva E Y 2021 *Combust. Sci. Technol.* 1–17
[2] Gurentsov E V, Eremin A V and Mikheyeva E Y 2017 *High Temp.* **55** 723–730