Studying the kinetics of the soot particles growth in the HACA mechanism

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The study of the growth mechanism of soot particles is still of considerable interest. Experimental data make it possible to obtain only grown structures or decomposition products of soot particles, however, the intermediate processes during the formation of nanostructures remain unclear [1,2]. Recent data [3] indicate the presence in the regions of soot formation of PAH molecules with masses of 180-600 daltons, which act as the initial reagents in the soot nucleation process. However, no less recent data [4] indicate that the concentration of PAHs in typical flames is insufficient to maintain the nucleation of soot—the authors, on the contrary, assign this role to benzene and lighter molecules. One of the methods for studying the growth processes of soot structures is the study of collisions between molecules under various conditions [2]. This paper presents the results of MD calculations with the ReaxFF potential for two incipient soot structures, similar to those presented in [3] and for acetylene and benzene molecules. Statistics were obtained on such collisions at different relative positions of objects in two temperature regimes: 500 K and 2000 K. The energy profiles of collisions were analyzed, the fraction of effective collisions and statistics on the collision time were calculated, and the influence of the local structure of a particle on these parameters was investigated.

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