

Effects of ambient CO₂ and H₂O on soot formation in n-dodecane spray combustion

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In this study, large eddy simulation (LES) is performed to investigate the effects of ambient carbon dioxide (CO₂) and water (H₂O) on the soot formation in an n-dodecane spray flame. A two-equation soot model, in which acetylene (C₂H₂) is set as the soot precursor and surface growth species, while OH is selected as the one of the soot oxidizers, is implemented here. The ambient oxygen (O₂) level and temperature are fixed at 15% (mole basis) and 900K, respectively. The predicted ignition delay, lift-off length, and soot distributions show good agreement with experimental data. The effects of ambient CO₂ and H₂O on the soot formation can be separated into thermal and chemical effects. For the thermal effects, the ambient CO₂ and H₂O enhance the formation of C₂H₂ but reduce the formation of OH radicals by lowering the flame temperature. This leads to a higher soot mass formed. Conversely, the ambient CO₂ and H₂O reduce the soot formation due to their chemical effects. The reaction $\text{CH}_2^* + \text{CO}_2 \leftrightarrow \text{CH}_2\text{O} + \text{CO}$ is found to be main pathway for reducing C₂H₂ formation when the ambient CO₂ is present. The ambient H₂O results in a lower C₂H₂ mass formed due to a higher amount of OH radicals produced. As a result, these collectively lead to a lower soot mass formed.