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Influence of Various Promotors and Inhibitors of Soot Formation on the Production of Soot Nuclei

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Abstract

Soot formation during pyrolysis and oxidation of rich mixtures of aliphatic hydrocarbons with single and multiple bonds in the presence of promotors (aromatic and metalorganic compounds) and inhibitors (hydrogen additives) of soot formation is experimentally studied behind reflected shock waves and simulated within the framework of a proposed kinetic mechanism. The influence of small additives of toluene to propane was demonstrated to substantially promote soot formation, whereas iron pentacarbonyl addition to propane and acetylene was shown to dramatically widen the temperature interval of soot formation both to higher and lower temperatures. Soot particles formed in the presence of iron pentacarbonyl gained magnetic properties due to the formation of an iron core inside the soot particle. The influence of acetone and propane additives to acetylene/argon mixtures was also studied. This is important to estimate the influence of impurities inherent to commercially manufactured acetylene. Hydrogen additives to acetylene/Ar mixtures were found to suppress the process of soot formation.

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Nomenclature

SY	soot yield
$E(m)$	optical absorption function
T_{50}	theoretical temperature behind a reflected shock wave
P_{50}	theoretical pressure behind a reflected shock wave
τ_{reac}	reaction time
TEM	transmission electron microscopy

1. Introduction

During the last few decades, experimental and modeling studies of nonequilibrium nanoparticle formation in various combustion systems have attracted an increasing interest of researches. Although the mechanisms of the formation of particulates, in particular soot, are not completely understood, the behavior of environmentally hazardous species has been computationally reproduced with an acceptable degree of accuracy. Soot is formed in flames under fuel-rich conditions due to incomplete combustion of the fuel, and burns out when mixed with the oxygen at high temperatures. As a result, soot formation is an essentially nonequilibrium process. In addition, the formation of soot nuclei is accompanied by a significant energy release, which leads to a substantial overheating of the nuclei relative to the surrounding gas-phase medium, thereby giving rise to a sequence of nonequilibrium reactions. There are two different stages of soot particle formation: the inception of particles (nuclei), from which soot is ultimately produced (nucleation process) and the subsequent growth of these particles which, in turn, takes place in two different stages, surface growth and agglomeration. Finally, soot represents the agglomerates of the primary spherical soot particles. The presence of additives in the reacting mixture, which promote or inhibit the nucleation process, can make this process even more nonequilibrium [1].

The influence of metal additives was studied in various combustion systems [2, 3]. Additives containing manganese, iron, and barium reduce soot formation in flames [4]. Iron pentacarbonyl also produces a significant flame inhibition effect [5]. In particular, in [6] it was demonstrated that iron pentacarbonyl [$Fe(CO)_5$] is one of the strongest inhibitors in flames. In [7], a review on flame inhibition by metal-containing compounds is presented. Several gas-phase kinetic models are described that explain the influence of inhibitors on laminar flames. The results of measurements of particles formed from the metal-containing species are analyzed, and the role of particles in flame inhibition by metals is discussed.

Such metals as iron, titanium, manganese, zinc, and chromium, are present in lubricant oils and diesel fuels. Induced soot nucleation due to an early condensation of metal oxides may occur over a cylinder volume. If the metal concentration is high enough, the induced nucleation can considerably promote the slower homogeneous nucleation via polycyclic aromatic hydrocarbon formation and growth. In [8], on the basis of qualitative considerations, two mechanisms were proposed of the influence of on soot formation. The first one involves the reaction of carbonyl fragments with the initial hydrocarbon or its reaction products to form small carbon–iron clusters and the promotion of H-atom production at early stages of the hydrocarbon pyrolysis. The second one is the fast formation of iron clusters with subsequent soot growth on the cluster surface.

The experimental data available in the literature show that depending on the experimental conditions, $Fe(CO)_5$ additives can either promote or suppress the soot formation process. In this connection, the main goal of the present work was to perform an experimental and simulation study of the effect of iron pentacarbonyl and other additives on soot formation during the pyrolysis of propane/argon and acetylene/argon mixtures behind reflected shock waves.

2. Experimental

The experiments were performed in a stainless steel shock tube (inner diameter, 75 mm; driven section length, 1.5 m; driver section length, 3.2 m). The details of the experimental setup are presented in [9, 11, 16]. The driver gas was helium. Mixtures (in mole %) of 1.66 C_3H_8/0.1 (or 0.3) $Fe(CO)_5$/Ar, 1.66 C_3H_8/1.0 O_2/Ar, 1.66 C_3H_6/Ar, 1.45 C_3H_8/0.1 C_7H_8 (toluene)/Ar, 5.0 C_2H_2/0.3 $Fe(CO)_5$/Ar, and 4.0 C_2H_2/1.0 C_3H_8/1.0 acetone/Ar additives were

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