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Paratherm-NF aerosol combustion behavior simulation: Ignition delay time, temperature distribution of flame propagation, and heat kernel hypothesis of combustion process analysis

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ABSTRACT

Aerosol combustion, especially for high-flash point materials, is a very complicated phenomenon inclusive of droplet evaporation, temperature increase, flame formation, flame propagation, and flame quench. A better understanding of a flame development can make this process clear to analyze, with possible mitigation system design according to the explanation of how the aerosol system gets ignited and how long it takes to form a harmful flame, which can propagate, accelerate, and cause fire or explosions. The authors of this paper have conducted a series of simulation regarding physical formula in description of this combustion process, and will conclude with how temperature distribution influenced the appearance of luminous flames, which was the symbol of successful ignition of aerosol. The novelty on this research is on the cutting point of flame appearance by setting of different temperature probes within aerosol system and determining various locations of testing, while more common studies have been done usually by means of existing flame expansion. Aerosol system in this paper was according to an electrospray-generated droplet group from experiments (Huang, Li, & Mannan, 2013) and trying to improve the explanation on the complex behavior for mixture materials with high flash point, which has not been done by other studies yet. We obtained the result that most of the initial heating time (~10–15 s after appearance of ignition source) is for turbulent heating on the closest, horizontal region of aerosol cloud; the next stage (~up to 40 s), on the other hand, has the determining force on vertical movement of the "heated kernel" as the new ignition source on fresh aerosols feed. The sustainable flame occurred after the delay time regarding the above mechanism. The mitigation implementing timing and location can also be characterized with further understanding of this combustion process, which is the functionality of our results in this fundamental analysis. The potential application of the ignition delay will be beneficial to the mitigation timing and detector sensor setting of facilities to prevent aerosol cloud fires.

1. Introduction

Aerosol droplets are formed from pressurized materials, such as accidental rupture, pipeline breakage, and storage unit corrosion. A common scenario of incidents would be the accumulation of an aerosol cloud to flammability limits of mist combustion, with a surrounding ignition source to make the initial flame appear. Some understandings of flammability have been studied in relatively highly flammable materials, such as iso-octane, diesel oil, n-decane, n-heptane, and methanol (Bowen & Shirvill, 1994; Atzler & Lawes, 1998; Hayashi & Kumagai, 1974; Myers & Lefebvre, 1986; Singh, 1986). Compared with gaseous flammable mixtures, data on aerosol flammability is rare. One reason for this is the huge complexity of the aerosol ignition process, and the difficulty of carrying out experiments with setups sophisticated enough to account for various factors in the process (Ballal & Lefebvre, 1981). Commercial heat transfer fluids, such as Paratherm-NF, Dowtherm-600, and many others, have a specific characteristic of high flash point to make them difficult to be ignited in pure liquid states. They are also hard to exist in pure gaseous state in process conditions, so the ignition and combustion data in vapor phase are still lacking. However, there are more than 200 reported incidents from the previous 20 years, which were considered to be related to heat transfer fluids in accidental leaking conditions. Aerosols formed by high flash point materials need to be studied to find a better explanation of the ignition, flame appearance, flame sustainability, and the mechanism of droplet combustion.

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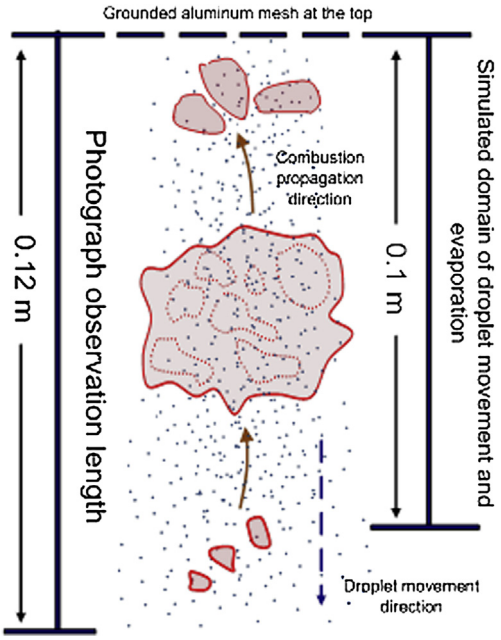

Fig. 1. The flame development stages of aerosol combustion (Peng et al., 2010).

Aggarwal (1985) analyzed the fuel spray ignition models, having found that the influential factors of the one-dimensional, monodispersed system ignition are the droplet size, ignition source temperature, cold gas temperature, initial fuel vapor concentration, distance between the hot wall and the nearest droplets, equivalence ratio, and fuel type. Those factors, as well as it affected the initial heat transfer to bring the energy for flame formation up to the fuel–vapor mixture further away, have potential influence on the combustion and flame propagation (Suard, Haldenwang, & Nicoli, 2004). Also, from the study of Lian, Mejia, Cheng, and Mannan (2010), we realized a phenomenon that the flame tends to starting by a series of small fragments, propagating upwards into the fuel-rich region where the streams of spraying are not deviated in directions due to an electric field. However, after these flame pieces form, there is a delay of time and distance before the huge global flame was formed. This "flame disappearance" region, about 4–6 cm in length, was thought to have relations to the further delayed ignition. The mechanism within this area has not been discussed in any kinds of aerosol or spray studies and remained unknown even though the delay of ignition was analyzed in other research.

In this study, we tried to adapt models used in energy materials coupled with the flame speed development process, which is based on the flame front propagation theory in aerosols, to the flame kernel growth model applied in spark ignition modeling for flammable mixtures (Lian et al., 2010). Other than the ignition energy input, we added the sub-model on droplet evaporation during the process of a "traveling heated kernel" (discussed in detail in section 2), and observed the flame appearance-to-quench procedure comparing to experiment results on the temperature distribution among this tested space, hoping to conclude a better model to predict the ignition delay and the timing for mitigation application in practical cases.

2. Simulation description

2.1. Model description

The process of aerosol stream combustion is shown as Fig. 1. This system is based on the cooperative aerosol project done at Mary Kay O'Connor Process Safety Center at Texas A&M University (Lian et al., 2010). P-NF is contained in syringes for spraying use. The method used to produce aerosols from liquid is electrospray, which is mainly the application of high voltage (up to 10 kV) onto the droplet streams, making the droplets charged and form minute droplet streams. These are the aerosol states defined in this study. The method was from a study of Mejia, He, Luo, Marquez, and Cheng (2009), introducing the electric control of the fine distribution of aerosol droplets. The size and space distributions can be varied by differently applied voltages and liquid flow rates. The liquid meniscus at the outlet of each capillary took a conical shape, *i.e.* cone-jet mode under the influence of the electric field between the nozzles and the grounding electrode (Lian, Mejia, Cheng and Mannan, 2010). The distance between the grounding electrode (attached to a metal mesh) and the nozzle front is 2.5 inches and remains the same for every test. The ignition source for the testing system is liquid propane gas or LPG flowing through a 1/8 inch inner diameter stainless steel tube. The inside end of the tubing was bent 90° up as the flame tip, so LPG gas would flow upward before being ignited upon exiting the tubing. The aerosol droplets traveled downwards with the ignition occurring at the very bottom of the chamber. The experimental setup is shown as in Fig. 2.

The whole procedure of the flame development in an aerosol system can be separated into three regions: (I) the flame pieces from the ignition source, (II) the global flame (which is the main

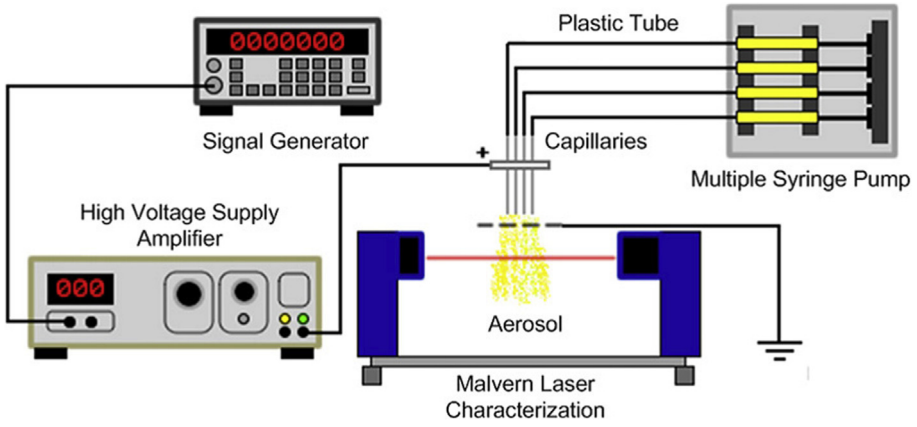

Fig. 2. Experimental setup for aerosol ignition study (Huang et al., 2013).