



Theoretical analysis and simulation of methane/air flame inhibition by sodium bicarbonate particles

Omar Dounia^{a,*}, Olivier Vermorel^a, Thierry Poinso^b

^aCentre Européen de Recherche et de Formation Avancée en Calcul Scientifique (C.E.R.F.A.C.S), France

^bInstitut de Mécanique des Fluides de Toulouse (I.M.F.T), France

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ABSTRACT

The capacity of sodium bicarbonate (NaHCO_3)_s powder to chemically reduce flame speeds and mitigate the effects of accidental explosions is well established. The inhibition of premixed hydrocarbon/air flames by monodisperse (NaHCO_3)_s solid particles is investigated, here, using theory and numerical simulations. First, an analytical solution for the temperature history of a solid (NaHCO_3)_s particle crossing a flame shows that the size of the largest (NaHCO_3)_s particle which can decompose inside the flame front, and act on chemical reactions efficiently, strongly depends on the flame speed. For various fuels and a wide range of equivalence ratios, particles with a strong potential for flame inhibition are identified: hence a criterion, on the maximum particle size, for efficient inhibition is proposed. Thereafter, a one-dimensional methane/air flame traveling in a premixed gas loaded with sodium bicarbonate is simulated using a chemical mechanism based on GRI-Mech, extended to include inhibition chemistry and reduced to 20 species with a DRGEP method (Pepiot-Desjardins and Pitsch, 2008). Inhibitor particle size and mass loading are varied to study the flame response to inhibition by (NaHCO_3)_s powders. Finally, two-dimensional simulations of a planar flame traveling in a flow with a non-uniform inhibitor mass loading distribution are analyzed. In the case of strong particle stratification, an acceleration of the flame is observed, instead of a mitigation. This fundamental mechanism may limit the actual potential of inhibition powders in real configurations.

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1. Introduction

Until the 1970s, industrial safety processes relied heavily on chlorofluorocarbon gases as fire suppressants in ground, sea and air systems [2]. Since then, the threat to Earth's ozone of such gases has been established and their production prohibited. Following this ban, intensive research has been conducted to find efficient halon replacements. Alkali metal compounds, such as sodium bicarbonate (NaHCO_3)_s have received considerable attention because of their higher effectiveness per mass basis compared to the halon 1301 (CF_3Br) [3]. Extensive experimental investigations on flame inhibition (reduction of flame speed) and flame suppression abilities of (NaHCO_3)_s demonstrate the effectiveness of these powders on premixed flames [4–7] and counter-flow flames [8–11]. More recent laboratory scale and medium scale (50 m³) experiments [12] show the capacity of alkali metal compounds to mitigate the potential aftermath of gaseous explosions.

The first systematic investigation of the mechanism of flame inhibition/suppression by (NaHCO_3)_s particles was performed by Rosser et al. [4]. The overall mechanism includes two major steps illustrated in Fig. 1: 1) thermal decomposition of sodium bicarbonate particles and 2) gas-phase chemical interaction with the flame.

1.1. Particle thermal decomposition

Exposed to a temperature gradient inside the flame front, (NaHCO_3)_s solid particles undergo thermal decomposition. Iya et al. [7] demonstrated that particles of (NaHCO_3)_s below 10 μm decompose completely inside the methane/air flame front. Chelliah et al. [11] also showed a monotonic behavior of suppression effectiveness with particle diameter for methane/air flames (contrary to the results of Trees and Seshadri [2] for heptane flames). These studies indicated that the particle size influences the position at which (NaHCO_3)_s decomposition is complete. Large particles, typically larger than 60 μm, will decompose too far downstream of the flame front leading to unsuccessful flame inhibition. The gas temperature decrease during this decomposition phase is generally negligible and does not modify the flame speed significantly.

* Corresponding author.

E-mail address: dounia@cerfacs.fr (O. Dounia).

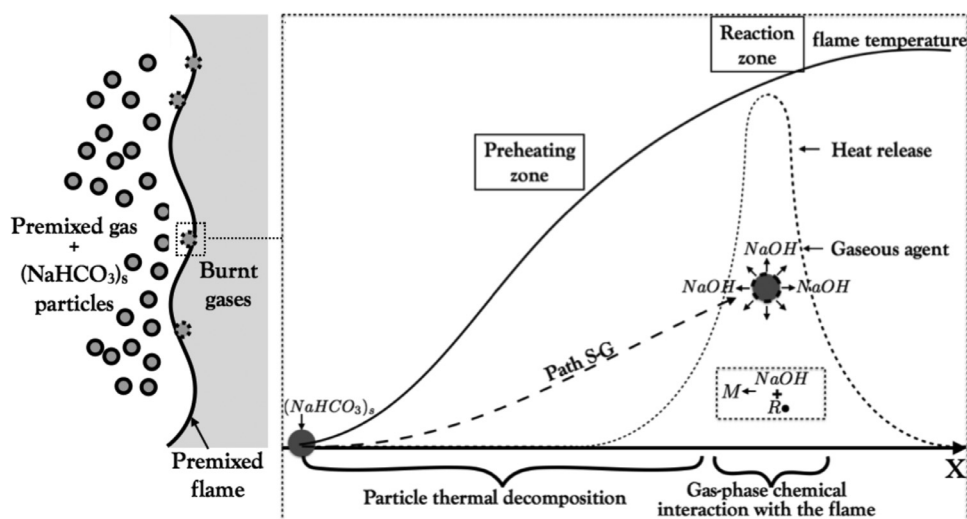
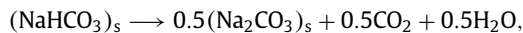


Fig. 1. Schematic of the flame inhibition mechanism by sodium bicarbonate. Path S-G refers to the path from the Solid bicarbonate particle to the Gaseous agent NaOH. $R\cdot$ stands for a radical species and M denotes a group of stable species.

1.2. Chemical interaction with the flame

The strong potential of sodium bicarbonate powders for flame mitigation is attributed to a chemical rather than thermal (cooling) interaction with the flame. Iya et al. [7] found a good correlation between the concentration of Na evaporated from salts and the degree of flame inhibition. They concluded that the mechanism behind flame inhibition by salts is chemical and homogeneous, i.e. taking place in the gas phase as a result of the presence of vaporized inhibitor. More recently Chelliah et al. [11] conducted experiments on the extinction condition of counterflow methane/air flames. Multiple particle size classes were considered. This study demonstrated the dominant chemical nature of flame inhibition by fine $(\text{NaHCO}_3)_s$ particles. Since flame inhibition by $(\text{NaHCO}_3)_s$ is due primarily to chemical effects, many authors [7,11,13–15] have proposed kinetic models based on NaOH being the main gaseous agent, able to act on chemical reactions in the flame. Gaseous sodium hydroxide (NaOH) is formed when the $(\text{NaHCO}_3)_s$ particles are exposed to high temperatures inside the flame front. The particles undergo thermal decomposition following a series of reaction pathways (path S-G in Fig. 1) leading to the formation of NaOH. The interaction of NaOH with the flame is homogeneous (gas-phase chemistry) and involves the catalytic recombination of the radical species responsible for the flame consumption speed, namely H, OH and O.

While the main product of the decomposition of the sodium bicarbonate is agreed upon, the path from the $(\text{NaHCO}_3)_s$ particle to the gaseous species NaOH (path S-G in Fig. 1) is still uncertain. Hu et al. [16] and Wu et al. [17] proposed a temperature range (370–543 K) and kinetic rates for the first stage of the thermal decomposition:



However, the following steps lack details and rates. In addition to the uncertainties surrounding $(\text{NaHCO}_3)_s$ decomposition kinetics, the influence of the powder injection procedure on the effectiveness of the inhibitor has not been addressed yet. In practice the methods used to deliver the powder to the gas can hardly guarantee a uniform particles distribution. A stratified or segregated powder can perturb the flame front and increase its surface, suggesting a possible opposite effect (increase in flame speed). This behavior was mentioned by Rosser et al. [4]: ‘In the absence of powder the flames were approximately hemispherical in shape; ... The pres-

ence of powder resulted at times in irregular flame shapes ... In some cases the flames were very long and highly tilted, probably as a result of non-uniform powder distribution’. More recently, various inhibitors, gaseous and liquid, failed the qualification test performed by the Federal Aviation Administration (FAA). The Aerosol Can Test (ACT) report [18] issued by the FAA showed that in some cases the overpressure increased in presence of inhibitor agents compared to the case with no agent. Even if the exact cause for these disappointing results is not identified, the powder segregation mechanism may explain it: in the context of vapor cloud explosions (VCE), the inhibitor injection would be performed through a discrete number of high pressure manifolds. Powder segregation is therefore unavoidable and may potentially lead to the amplification of VCE damages. This possibility clearly requires additional studies if such mitigation systems are used in the future.

The present work describes a theoretical and numerical study of the influence of sodium bicarbonate powders on flame propagation. The first objective is to derive a model (HetMIS) for the Heterogeneous methane/air inhibition by Sodium bicarbonate suited for numerical simulations in large and complex configurations. HetMIS is composed of: 1) a simplified 1-step model for particle decomposition (Section 2.1); 2) an analytically reduced chemistry (ARC) for flame-NaOH interaction (Section 2.2). The introduction of complex chemistry using ARC schemes [19–22] is mandatory to capture the chemical effects of NaOH on the flame at a reasonable cost. An analytical expression for particle temperature is derived in Section 3 to predict where particles decompose in a premixed flame, hence to propose criteria on particle size for complete decomposition inside the flame front. Based on these criteria, a selection of particle sizes is used to study the effect of sodium bicarbonate powder on the propagation of a 1D flame (Section 4). Finally, the response of a planar flame to a non-uniform distribution of sodium bicarbonate particles is examined in Section 5 using two-dimensional simulations to show that the local flame speed reduction can be offset by a flame surface increase when the distribution of inhibitor is not homogeneous.

2. Model for Heterogeneous methane/air flame Inhibition by Sodium bicarbonate (HetMIS)

The HetMIS model includes a simplified description of the particle evolution from solid $(\text{NaHCO}_3)_s$ particles to gaseous NaOH

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