Mitigation of Strong Deflagrations by Water Mist

M. Teresa Parra, Francisco Castro, César Méndez, José M. Villafruela
University of Valladolid, Spain

Corresponding Author, M. Teresa Parra: terpar@eis.uva.es

Introduction

The present numerical work focuses on the interaction of a premixed flame and a water mist in order to provide its mitigation. Propagation occurs in a confined domain of high length and reduced transversal area, which provides the appearance of pressure waves that accelerate the flame front. The extinction criteria based on the flame propagation velocity and the Damköhler are analyzed.

Water spray barriers of fine droplets can be very effective in quenching strong flames (Grant 2000). When water droplets change from liquid to steam, there are important reductions of temperature and oxygen concentration in the flame front surroundings. Droplets must be large enough to avoid the drag and small enough to evaporate quickly. Optimum water droplet sizes ranges from 50 to 200 microns of mean diameter.

Numerical model

This section presents a brief summary of the code SECIBA (Simulator of Confined Explosions and its Interaction with Barriers of Water) developed by the authors to carry this research out. Readers should examine reference (Parra 2004) for an extensive description of the SECIBA code.

A confined domain of 18 m of length and 1.5 m high has been simulated, figure 1. To simulate the hot spot ignition, the initial temperature is 1800 K on the closed side of the domain. The initial concentrations correspond to a stoichiometric methane/oxygen mixture in air. The water barrier of 50 μm droplets size and 0.05 % liquid volume is located from x = 3m to the end of the domain.

![Figure 1. Scheme of the numerical model](image)

The gas flow behaves according to the Euler equations expressed for a two-dimensional, transient, compressible and reactive flow. A simplified reaction mechanism, result of a sensitivity analysis (Warnatz 1996), is employed. The use of an adaptive mesh provides a method of pressure capture. Because of the characteristic time of the chemical reactions is small relative to the time step length of the convective transport, it is necessary to use a time splitting technique. The conservative equations are solved using the Flux Corrected Transport...
algorithm developed by Boris, (Gross, 1985). The chemical kinetics use the CHEMQ solver developed by Young (Oran, 1987) to evaluate the chemical species concentrations. Monodispersed water barrier is modeled by an eulerian description. Main interaction effects of the gas mixture on the water droplets are drag, break-up, heating and vaporization of the water droplets (Sirignano 1993). The interaction between liquid and gas phases is represented by source terms.

**Influence of the water barrier on the gas mixture behavior**

The figure 2 shows the pressure evolution for the adiabatic flame and the flame interacting with a water barrier located at 3 m from the ignition region. When the flame interacts with the water barrier, the peak of pressure goes up slower than these of the adiabatic flame. Therefore there is a decrease of the propagation velocity.

![Figure 2. Pressure profiles for an adiabatic flame and a flame in presence of the water barrier](image)

Figure 2 presents the temperature profile and the mass fraction of the fresh mixture for the adiabatic and the perturbed flames. They are plotted at different instants of time in order to have the flame front at a similar location. The weak gradient of temperature and the reactive components on the perturbed flame is consequence of the slowdown of the reaction rates. The presence of steam produces a significant modification of the mixture composition as well as a
decrease of the temperature of the mixture. Note that the specific heat of the steam is bigger than the one of the gas mixture.

**Influence of the gas mixture on the water barrier behavior**

Figure 4 shows the flame front and the pressure wave position for the perturbed flame. It is clear both are decoupled and the pressure wave is responsible of the drag of droplets to downwind sections. Eötvös and Weber numbers indicate that the main break-up agent is the instantaneous acceleration instead of the relative velocity. The boiling regime begins after the breakup because small droplets have a high surface/volume ratio and reach very quickly the saturation temperature.

![Figure 4. Temporal evolution of the flame front, pressure wave, drag of the droplets and their chronological regarding the regimes of heating, boiling and breakup.](image)

**Extinction criterion based on the Damköhler number**

The extinction criteria depend on the propagation velocity of flame front. So that, criteria of deflagration mitigation can be expressed as function of reaction kinetics parameters, but detonation’s mitigation conditions can be expressed in terms of energetic considerations. Chao and Law found out that a lean premixed methane-air flame is mitigated when its burning rate is lower than 60% of its corresponding adiabatic rate. (Bechtold, 1994).

Combustion is governed by phenomena of different nature, such as diffusion and convection and chemistry. The relative importance of the chemical reaction with reference to the remaining events is measured by a dimensionless parameter known as the Damköhler number. This is defined as the ratio of timescales associated to fluid-dynamic and chemical phenomena. Low Damköhler numbers characterize quasi-inert flows whereas high Damköhler values are associated with fast chemical reactions. There are different Damköhler number definitions, it has been used the Damköhler number 3:

\[
\text{Da}_3 = \frac{\text{Reaction Heat Flux}}{\text{Convective Heat Flux}} = \frac{Q L}{\rho U c T} 
\]  

(1)

Figure 5 shows that only water barrier with droplets sizes smaller than 100 μm are efficient to mitigate the flame according the Chao and Law criterion. In addition, the Damköhler number of the flame front on the steady regime is one order of magnitude smaller than this of the adiabatic flame.
Figure 5. Influence of the droplet diameter on the flame velocity and the Damköhler number (water barrier of 0.05 % liquid volume located at 3m from the ignition region)

Conclusion
The interaction of a monodispersed water barrier of droplets with a premixed methane/air flame that propagates in a confined domain has been simulated. The main interaction agents taken into account are the vaporization, drag and the breakup. An extinction criterion based on the Damköhler number is analyzed as well as the conventional criterion of the propagation velocity. The analysis reveals the important decrease of the flame propagation velocity for small droplets.

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